

PRO/II™ Process Engineering Air Separation Plant Casebook



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Case 1: Air Separation Plant

Abstract

The production of nitrogen and oxygen is an essential step in many chemical processes. These two gasses are the first and second most used industrial gases respectively.¹ Nitrogen is commonly used as a blanket gas while Oxygen is used in various processes because of its reactivity. Argon can also be recovered in air separation plants and Argon is commonly used as an inert filler gas. Due to high demand for these three gasses industrially, separating these components from air can be quite profitable if the plant is designed and operated efficiently.

Computer simulation is an essential tool in the design of new air separation plants and in modifying existing designs to meet new operating requirements. This casebook demonstrates the use of PRO/II in the simulation of an air separation process with Nitrogen, Oxygen and Argon products. This simulation includes pre-cooling the air and the use of a turbo-expander to produce the refrigerant.

This process contains one material recycle and a number of thermal recycles.

Since this process involves separating components with relatively close boiling points at very low temperatures. Special thermodynamics will need to be used to predict the separations accurately.

Introduction

Air separation is a commercially important process because both Oxygen and Nitrogen are essential materials in today's process industries. The main constituents of air are Nitrogen and Oxygen with a small amount of Argon. There are also traces of other rare gasses but these are only present in ppm.

Oxygen

The steel industry is the largest consumer of industrially produced Oxygen. Oxygen is injected into furnaces allowing more efficient combustion than air. The manufacture of chemicals is the second largest use of industrially produced Oxygen. The manufacture of ethylene oxide, acetylene, titanium dioxide, propylene oxide and vinyl acetate all require Oxygen. The chemical industry also uses industrial Oxygen for partial oxidation processes such as ammonia and methanol production.

Other uses for the industrially produced Oxygen include: coal gasification and liquefaction; oxy-acetylene welding; non-ferrous metallurgical processes; waste water treatment; and medical applications.

Nitrogen

Most of industrially produced Nitrogen is used as a gaseous blanket to exclude Oxygen and moisture. This may be to reduce explosion hazards in hydrocarbon liquid storage or to avoid corrosion with liquids such as sulfuric acid.

In the metals industry, Nitrogen is used as a blanket to prevent oxidation of the metal during smelting and to cool and purge molds of Oxygen before pouring in the metal. Nitrogen is also used in the oil exploration industry to enhance oil recovery by maintaining the pressure in the wells, while liquid Nitrogen is used to fracture the production section of oil wells.

A rapidly growing area for the use of Nitrogen is the electronics industry which uses about 15% of current production. Very high purity Nitrogen is used to provide an inert, dust-free, environment for the production of complex miniature components.

Liquid Nitrogen is widely used in cryogenic applications such as: food freezing and refrigeration; low temperature metal treatment; shrink fitting of parts; the storage of biological materials such as blood and organs; and in cryosurgical procedures.

The Nitrogen must be dry and have low Oxygen content. The amount of Oxygen allowed depends on the application and some typical values are shown in the following table.

Table: Nitrogen Purities for Various Applications

Application	Phase	Purity (ppm Oxygen)
Refineries, hydrogen storage blanketing	Gas	500
Pharmaceuticals, food and drink	Gas & Liquid	1 – 200
Electronics	Gas & Liquid	0.5 – 100
Well fracturing	Liquid	1 – 10

Argon

The steel industry is probably the largest user of Argon because of its inert properties. It is used to remove Oxygen from molds in pressure die-casting and to protect the molten metal in continuous casting.

Argon is also widely used as a high-grade inerting medium in welding in order to prevent oxidation at the welded joint. It must be used in preference to Nitrogen in high quality aluminum welding to avoid the formation of nitrides.

Other uses of Argon include: fill gas for light bulbs; gas chromatography; and as an inert medium or carrier gas in the production of semiconductors.

Manufacture

The vast majority of Nitrogen, Oxygen, and Argon are produced by the cryogenic separation of air. Nitrogen may also be separated from Oxygen by the combustion of hydrocarbons in air. This process, which also produces carbon dioxide, does not produce the same high purity Nitrogen as cryogenic separation and is much less common today. Oxygen can also be obtained by the electrolytic dissociation of water but this is expensive and virtually all Oxygen is produced from air separation. A small amount of medium purity (90-95%) Oxygen is produced by pressure swing adsorption processes but cryogenic separation is the predominant method. This is because, in addition to allowing the production of large quantities of high purity Oxygen, cryogenic processes can produce Oxygen as a liquid.

Virtually all Argon is produced from the cryogenic separation of air processes. A small amount of Argon is also produced as a by-product from ammonia synthesis. The purge drawn from the synthesis loop contains up to 6.5 mole % Argon which may be recovered by cryogenic technology.

The configuration of a cryogenic separation process depends on which products are to be made together with the phases and purities required. In small plants which supply only Nitrogen or Oxygen, the separation is usually carried out in a single distillation column. However, in larger plants, the use of a single column is generally inefficient.

Large plants must produce both Nitrogen and Oxygen in order to be economically viable, necessitating a double column configuration. Double column processes employ pressure difference to allow energy integration between the columns.

Argon has a boiling point between those of Nitrogen and Oxygen; therefore, it can build up within the distillation columns. It is removed as a side draw into another distillation column where it is removed as an overhead product. The remaining gases are returned to the Nitrogen/Oxygen separation column. Because of the increasing demand for Argon, more and more air separation plants now incorporate Argon recovery.

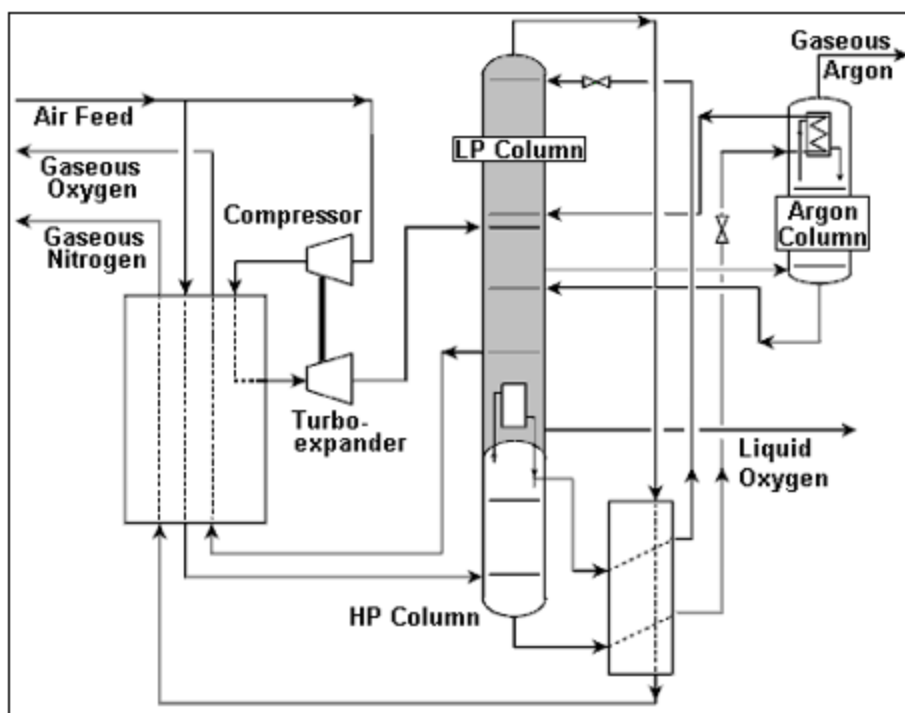
Most air separation plants can produce only small amounts (0-10%) of the products as liquid. If more liquid products are required, additional refrigeration must be supplied. If the plant is to produce predominantly liquid products, a liquefier can be integrated into the process at the design stage. Alternatively, a separate liquefier may be added later to liquefy Oxygen or Nitrogen products in the future as market conditions require.

The size of separation plants can vary considerably. Small plants will produce less than 0.1×10^6 kg/day of Oxygen whereas large plants may produce up to 2.2×10^6 kg/day.

Process Overview

The separation process in this casebook produces gaseous Nitrogen, Oxygen and Argon products. Part of the Oxygen is also produced as liquid. The plant produces approximately 1.5×10^6 kg/day of Oxygen between the liquid and gaseous phases. The flowsheet is illustrated below in the figure.

Figure: Air Separation Flowsheet



The separation of Oxygen and Nitrogen is carried out in a double distillation column. This consists of two separate columns which are physically placed one on top of the other. The bottom column (HP column) operates at higher pressure and its condenser is the reboiler for the upper, lower pressure, column (LP column). The HP column bottom product is fed to the LP column as feed and the reflux to the LP column is provided by the liquid top product from the HP Column.

The Argon column takes a vapor side draw from the LP column and returns its bottom product to the tray below the draw. The Argon product is drawn overhead.

Feedstocks and Products

Feed

Ignoring the impurities and traces of rare gasses, the composition of dry air feed is listed in the following table.

Table: Air Composition

Component	Mole %
Nitrogen	78.11
Argon	0.93
Oxygen	20.96
Well fracturing	Liquid

Products

Since the main use of Nitrogen is to exclude Oxygen, the Nitrogen produced in the air separation plant must contain very little Oxygen. This can range between 0.5 to 5000 ppm depending on the intended use of the Nitrogen. In this study, the amount of Oxygen in the Nitrogen product must not exceed 10ppm. Impurities in the Oxygen product are not as tightly controlled but the purity must be greater than 99.5%.

Argon, which is also used to exclude Oxygen, is also limited in the amount of Oxygen that it can contain. However, the relative volatility of Argon to Oxygen is about 1.1 at the top of the Argon column making it impractical to remove all the Oxygen by distillation. If the columns are efficient, the Argon product contains 0.5-1% Nitrogen with an Oxygen content of 1-2%. The Argon is then further treated by catalytic deoxygenation where the remaining Oxygen is burned with hydrogen.

Feed Pretreatment

The air used in the separation process must first be dried and other impurities removed. The impurities will include carbon monoxide, methane, ethane, ethylene and acetylene. Other impurities may be present depending on the location of the plant.

There are two basic methods for removing the impurities before the separation process:

- Chilling with Freon followed by molecular sieve adsorption;
- Using reversing exchangers to alternately freeze and sublime the impurities.

Molecular sieves are generally used in small plants while large plants (over 0.5×10^6 kg/day) generally use reversing exchangers as these have a lower pressure loss. However, molecular sieves are now becoming more common in larger plants.

Air Refrigeration

The normal boiling points of Nitrogen and Oxygen are 77K and 90K respectively. This means that the air must be cooled to very low temperatures for the separation. The air feed is cooled as much as possible by exchange with the gaseous product streams but additional refrigeration is required to compensate for heat loss and the production of liquid products.

Small plants provide the refrigeration by compressing the air to high pressure (typically 150 atmospheres) and using the Joule- Thomson effect to cool it as it expands through a valve. In large plants, the compression costs become too high for this to be economic. These plants only compress the feed air to about 6-8 atmospheres. The feed is split and about 10% is compressed, cooled and passed through a turbo-expander. The work produced by the expander is used to drive the compressor.

High Pressure Column Overview

The main air feed enters the HP column which operates at a pressure of approximately 6 atmospheres. The column separates Nitrogen from Argon and Oxygen, producing a pure liquid Nitrogen product overhead. This product contains a few ppm Oxygen with less than 0.2% Argon. If a liquid Nitrogen product is required from the process, it is drawn from the top of the HP column.

The flowrate of the bottom product from the HP column is about 60% of the feed rate and it contains about 35% Oxygen, 1% Argon with the remainder being Nitrogen.

Low Pressure Column Overview

The LP column operates at about 1.5 atmospheres and separates the Nitrogen and Oxygen to give pure products of each. The lower pressure gives better separation as it increases the relative volatility between the Nitrogen and Oxygen. The overhead product is gaseous Nitrogen with the same purity as the liquid Nitrogen product from the HP column. Both liquid and gaseous Oxygen are drawn from the bottom of the column. The Oxygen product stream

will be better than 99.5% pure because the Argon is removed from the side draw.

The main Oxygen feed to the LP column is the bottom product from the HP column. It is subcooled by exchange with the low pressure Nitrogen product and is used to provide the cooling in the Argon column condenser. It then enters the LP column with a liquid fraction in the region of 50%.

The air from the turbo-expander is fed a few trays below the main feed.

The reflux in the LP column is supplied by the liquid Nitrogen product from the HP column. This stream is subcooled by exchange with the low pressure Nitrogen product and flashed through a valve to give a 90% liquid reflux.

Argon Column Overview

The Argon column feed is a vapor side draw from the bottom section of the LP column and the Argon vapor is removed overhead. Because Nitrogen is more volatile than Argon, any Nitrogen in the feed will leave in the Argon product. It is therefore essential that the feed contains very little Nitrogen. In order to ensure this, the draw from the LP column is taken a few trays below the maximum Argon concentration. The draw rate is about 20% of the air feed rate to the plant and only about 4% of the draw stream is removed as Argon product.

Energy Integration

The process has a high level of energy integration as all the cooling is supplied from the feed pressure. There is no other refrigeration in the process. The main air feed is cooled to its dew point by exchange with the product streams. These streams are also heated by the product from the compressor. The compressor is driven by the expander and so its work also derives from the feed stream pressure.

The pressures in the LP and HP columns are set to ensure that the HP column condenser can provide heat for the LP column reboiler. This means that the pressure in the HP column must be sufficient to raise the overhead temperature 2-3K above that of the LP column bottoms.

The cooling in the Argon column condenser is provided by the HP column bottom product. The pressure is let down to ensure that its temperature is below the Argon column top temperature.

The HP column products are both liquid and supply the reflux in the LP column. As the pressures are reduced, they will vaporize thereby reducing the available reflux. The LP column overhead product is used to subcool these products to reduce the vaporization, and subsequent loss of available reflux.

Material Recycle

This flowsheet contains only one material recycle - between the LP and Argon columns. The flow in these streams is large compared to the product produced in the Argon column. It consists of about 90% Oxygen with the remainder mostly Argon. The draw from the LP column contains approximately 0.01% Nitrogen.

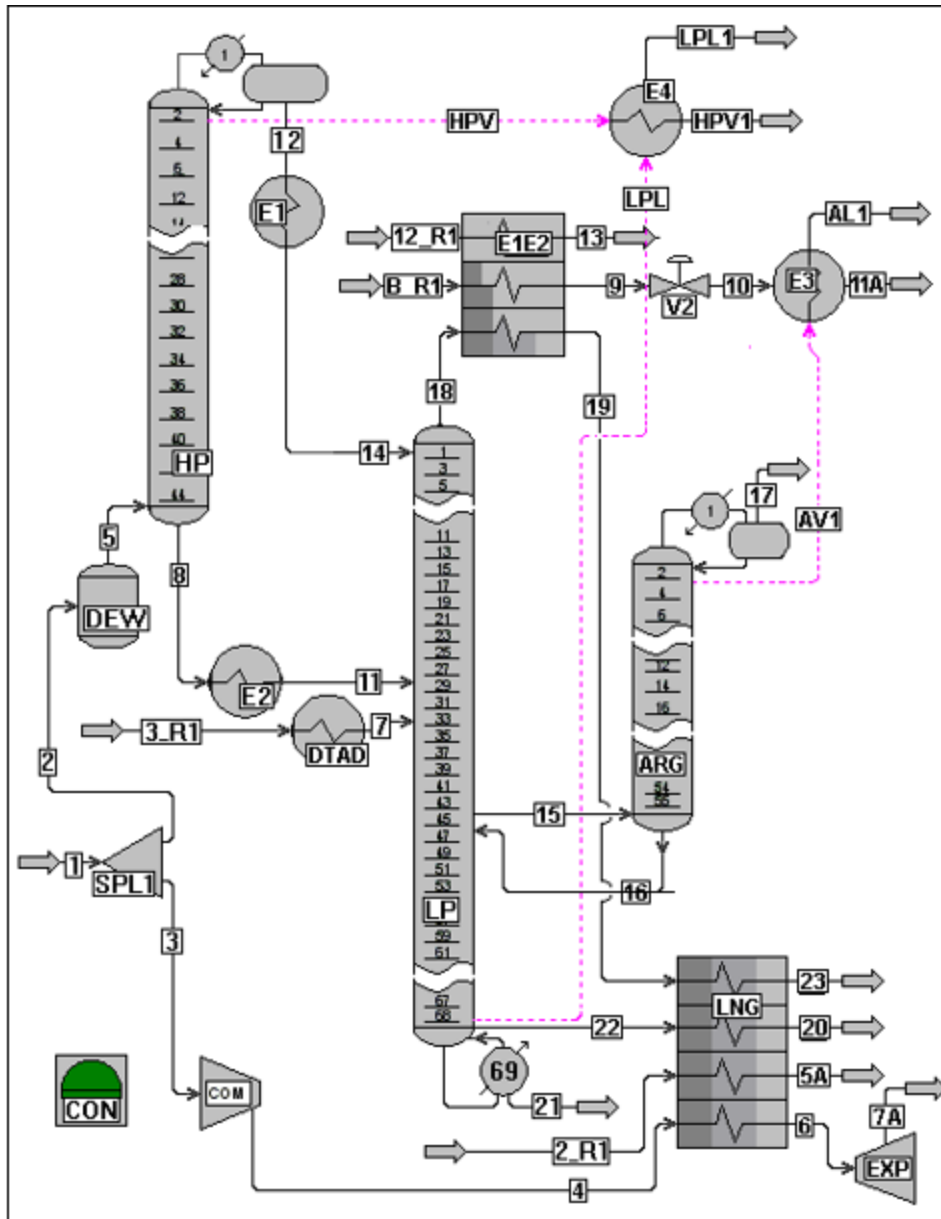
Process Simulation

Air Plant Flowsheet

The flowsheet illustrated in the following figure was adapted from the flowsheet PFD generated by PRO/II for the air plant simulation. It was edited only to fit the size and aspect ratio restrictions of this manual while still displaying readable labels. It differs from the process flowsheet that it includes stream identifiers and shows the unit operation icons actually used to simulate and solve the flowsheet. Screenshots of the PRO/II PFD are in *Simulation Flowsheet* on page 29. Selected results are listed in *Selected Output* on page 33.

The full input file for the simulation may be found in *Keyword Input File* on page 41. Screenshots of the important data entry windows that were entered in the graphical user interface appear within the text below.

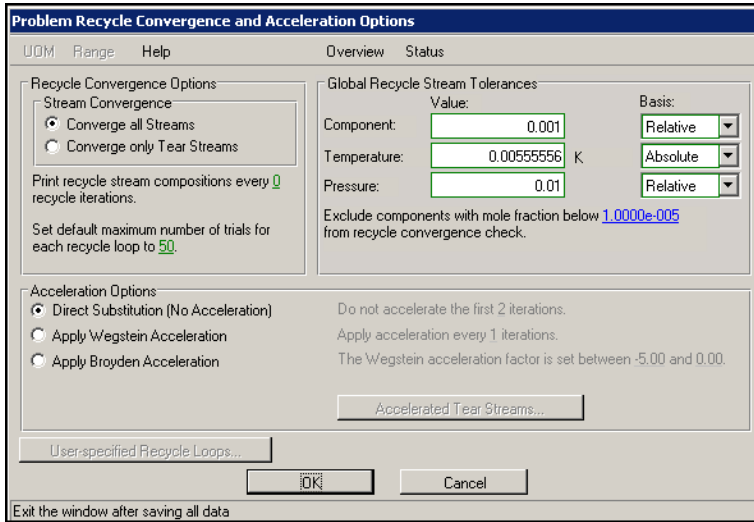
Figure: Representation of Air Plant Flowsheet



General Data

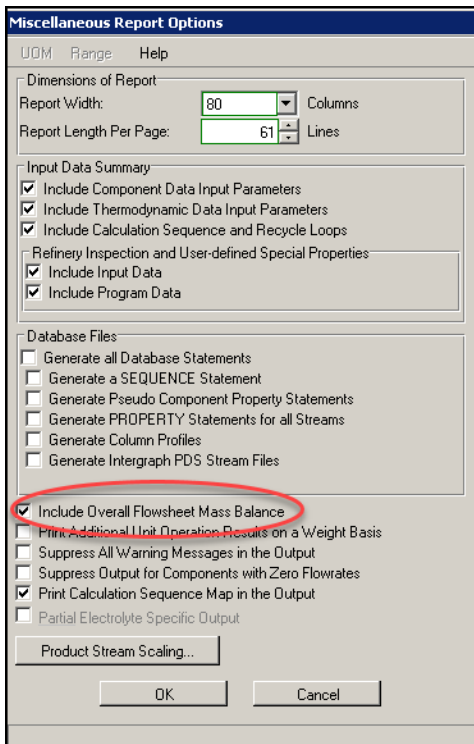
There is a recycle between the LP column and the Argon column. The threshold mole fraction limit for trace components is reduced to 1.0×10^{-5} because the Nitrogen concentration in the recycle is small. Using the default setting of 0.0, the Nitrogen balance would not be checked in the convergence test.

Figure: Recycle and Acceleration Dialog



By default, PRO/II includes the overall flowsheet mass balance in the output report. This may be controlled from the Miscellaneous Report Options screen.

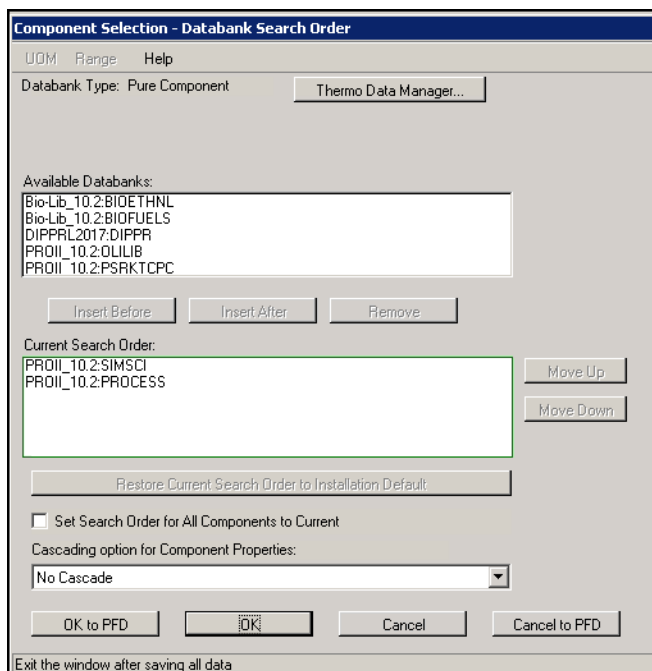
Figure: Miscellaneous Report Options



Component Data

All the components in the simulation are available in the PRO/II databanks. Note PRO/II includes several component data libraries including the Process and Simsci libraries that contain different versions of data for many components. The libraries are search in a user-specified order, so different data may be used depending upon the search order. Starting with version 8.0, the default search order is Simsci then Process. To obtain the same results as earlier versions of PRO/II, change this order to Process then Simsci.

Figure: Changing Component Bank Search Order



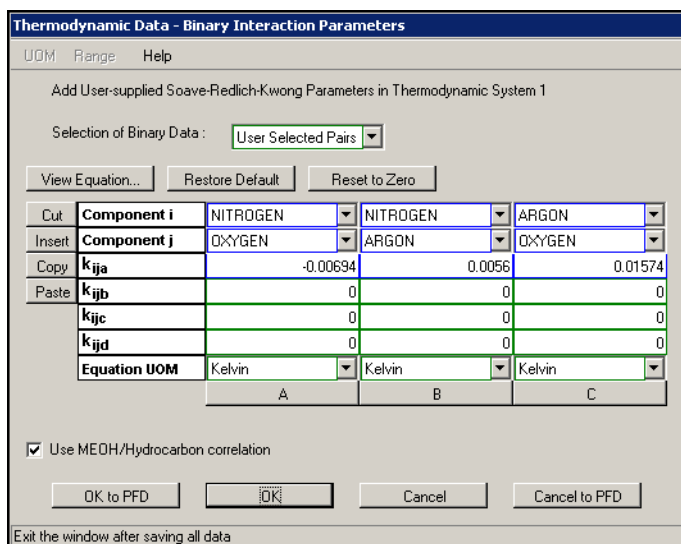
Thermodynamic Data

The importance of accurate thermodynamic calculations for this simulation can not be overemphasized. The product purities are specified in terms of parts per million and product temperature differences are only a few degrees. Any inaccuracies in the thermodynamic calculations will, therefore, have a significant effect on the results.

The Soave-Redlich-Kwong equation of state is suitable for the equilibrium, enthalpy and vapor density calculations for light gasses such as those in this simulation. Ideal liquid densities are used as they give better results for these components than the default API method.

The boiling points of Nitrogen and Oxygen are only 13K apart and those of Nitrogen and Argon are only separated by 3K. It is therefore essential to use binary interaction parameters obtained near process conditions for each pair of components in order to obtain an accurate simulation model.

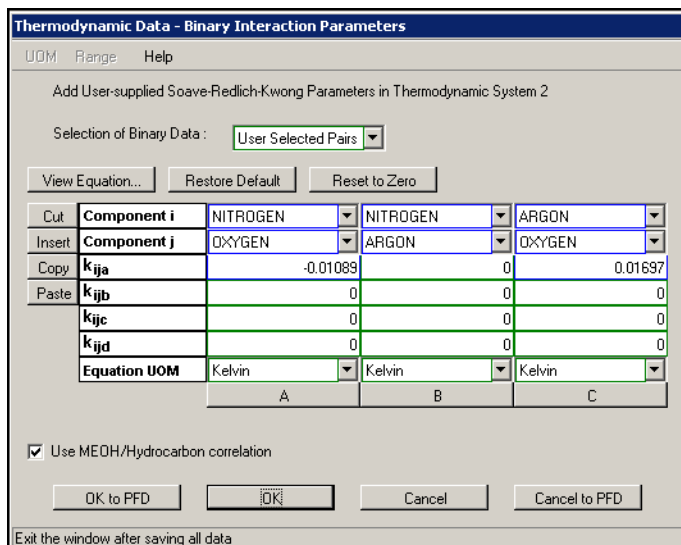
Figure: Low Pressure Binary Interaction Coefficients



The SIMSCI databank provides interaction parameters which cover a wide range of temperatures and pressures. For more accurate results, parameters should be derived for the specific temperature and pressure ranges in the simulation. The best source of these parameters is always in-house data, if available. Most companies who work with these plants will have derived interaction parameters in the past. If data is not available in-house, parameters may be obtained from the literature or by regressing experimental vapor-liquid equilibrium data.

This simulation uses separate interaction data for the high and low pressure sections of the process. The Nitrogen/Oxygen and the Argon/Oxygen interactions were obtained by regressing data for the specific pressure range from Gmehling & Onken (*Reference: Recommended Data of Selected Compounds and Binary Mixtures, Parts 1 and 2, 1987, DECHEMA Chemistry Data Series, Vol, IV, Stephan, K., ed., DECHEMA, Germany*). The low pressure Nitrogen/Argon parameter is the Gmehling & Onken regressed values. The binary interaction parameters used in the low pressure thermodynamic method, 1, are shown above in figure **Low Pressure Binary Interaction Coefficients**.

Figure: High Pressure Binary Interaction Coefficients



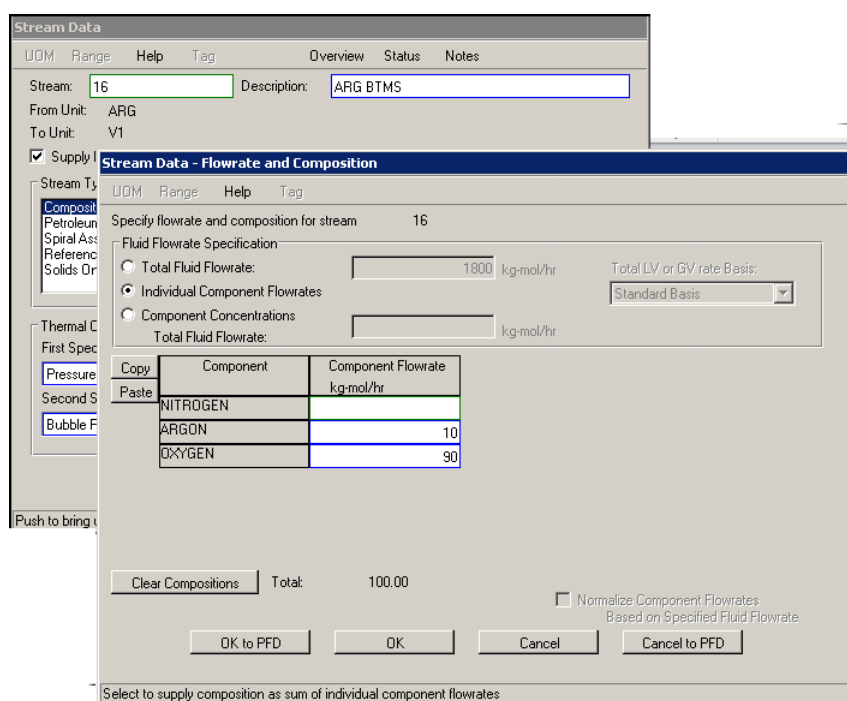
For the high pressure column, the Nitrogen/Argon interaction is assumed ideal and is set to zero. The high pressure binary interaction parameters used in the high pressure thermodynamic method, 2, are shown in figure **High Pressure Binary Interaction Coefficients**.

Stream Data

There is only one feed stream to the process which is the air feed. It comes from the purification stage where the water and carbon dioxide are removed. The temperature is 278K.

There is a recycle (stream 16) between the Argon column and the LP column. The recycle is named ARG BTMS. The following figure shows the initial estimate data input for this stream.

Figure: Initial Estimate Data for Recycle (Stream 16)



An initial estimate must be supplied because the Argon product flowrate is low compared to the return stream - about 4% of the feed. If the return stream is not known, then its flowrate can be estimated as 20% of the feed air flowrate and it is about 90% Oxygen with the rest consisting of Argon.

Calculation Sequence

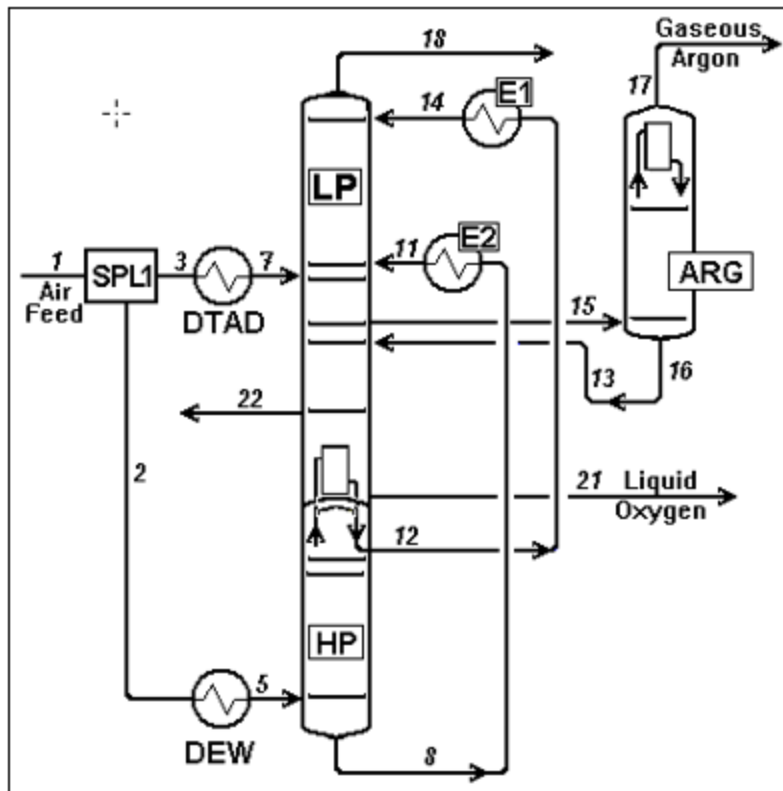
PRO/II handles the calculation sequence automatically by using the Minimum Tear Stream method. PRO/II solves this flowsheet by starting with the distillation columns rather than following the air feed stream through the process because the cold stream temperatures into the exchanger are unknown. However, the feed to the HP column is set at its dew point and the air feed to the LP column is 5K above its dew point.

The calculation starts at the HP column. After it is solved, the products streams are set to the correct pressures and liquid fractions for the LP column feeds and the LP and Argon columns are solved along with the recycle. After the recycle is solved, all of the other units can be solved.

Column Section

The column section includes not only the three distillation columns, but also the feed splitter and the exchangers to set the feed conditions for the feed streams to both the HP and LP columns. The flowsheet is shown in the following figure.

Figure: Column Section of Simulation Flowsheet

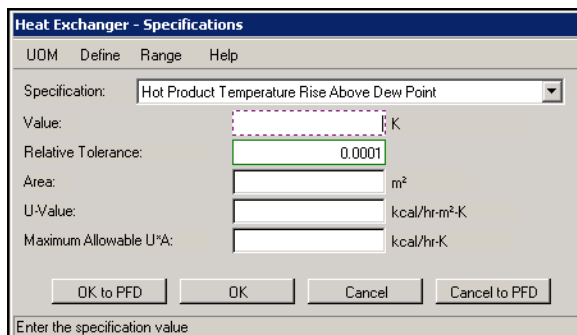


Feed Temperatures

Feed Temperatures

Ten percent of the pretreated air feed goes to the LP column via the compressor and expander. The remaining 90% goes to the HP column. The splitter divides the air feed and the products are set to the column inlet conditions. The feed to the HP column is set to its dew point at the inlet pressure in a flash. Heat exchanger DTAD sets the air fed to the LP column at 5 Kelvins above its dew point at a pressure of 1.4 atmospheres.

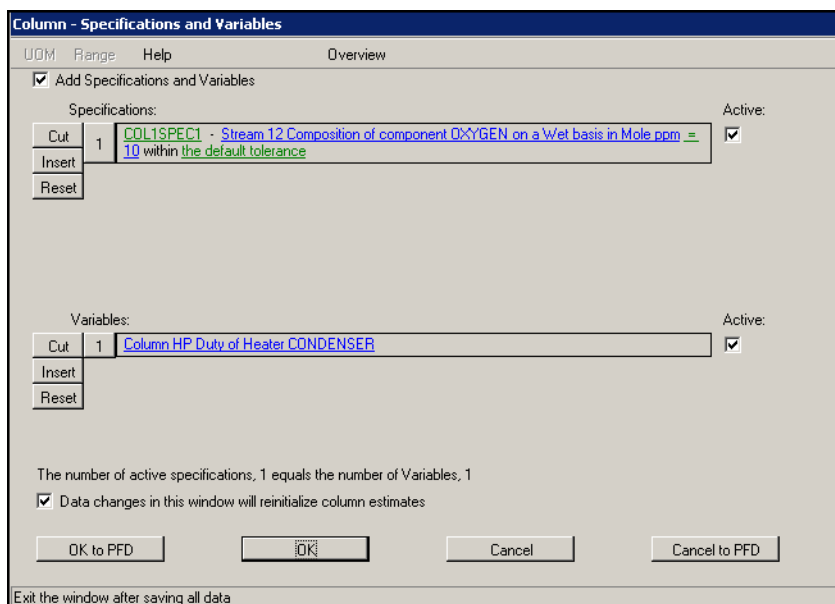
Figure: HP Feed Specification in Heat Exchanger DTAD



High Pressure Column

The HP column has a total condenser and no reboiler. The air fed to the base of the column acts as the reboiler. The only variable is the condenser duty, and it is varied to meet the 10 ppm Oxygen specification in the overhead product. A slightly edited image of the specification Data Entry Window is shown in the following figure.

Figure: HP Feed Specification in Heat Exchanger DTAD

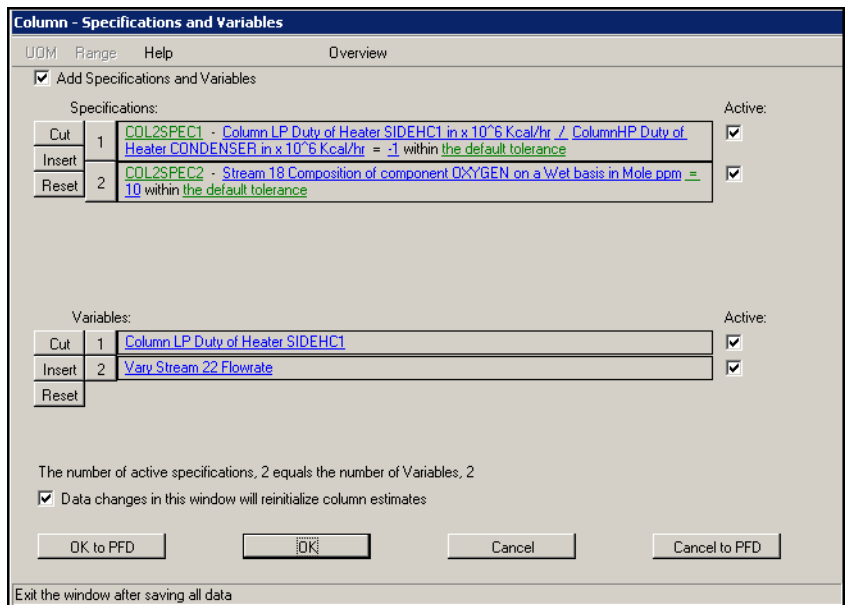


If the overhead product rate is not known, it can be estimated as 40- 50% of the feed. The thermodynamic method for this column is the high pressure method, 2.

Low Pressure Column

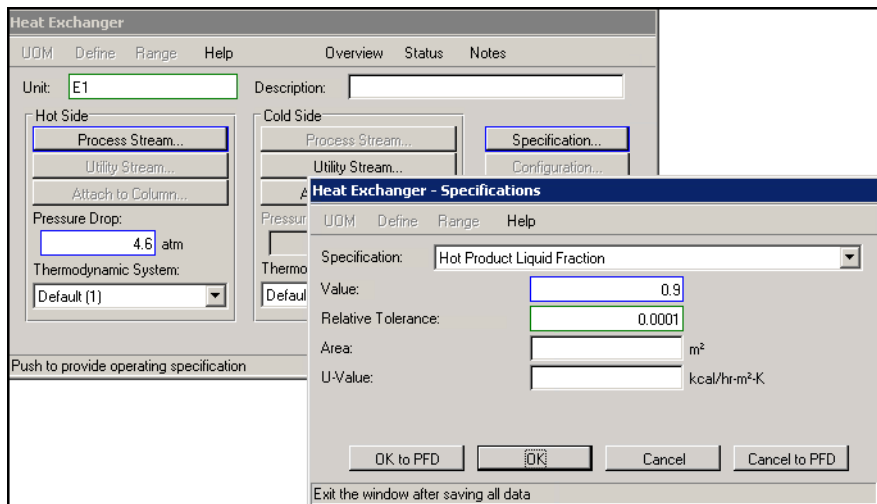
The products from the HP column are cooled by exchange with the overhead product before being fed to the LP column. The bottom product from the HP column also provides the condenser duty in the Argon column. When the LP column is calculated, the overhead product and the Argon condenser duty are not known and so the exchangers cannot be modeled at this time. Instead, the column feeds are simply set to the desired pressure and liquid fraction in heat exchanger models. The detailed exchangers are modeled later when the distillation columns have been solved. The thermodynamic method for this column is the low pressure method, 1. The slightly edited LP column specifications DEW is shown in the following figure.

Figure: Low Pressure Column Specifications



Heat Exchanger E1 specifications are shown in Figure 1-13: Similar data is supplied for exchanger E2, with pressure drop set at 4.55 atm and hot liquid product fraction set at 0.450.

Figure: Heat Exchanger E1 Specifications



The pure Nitrogen product from the HP column acts as the reflux and there is no condenser. This stream should be the same purity as the required product from the LP column. The HP column bottom (Oxygen) product enters in the top section of the column with the air feed from the turbo-expander a few trays lower down.

The Argon column draw and return are in the bottom section of the column. The products are Nitrogen overhead and Oxygen from the base. The Oxygen is mainly gaseous but a small amount of liquid Oxygen is also produced.

The reboiler for the LP column is the condenser for the HP column and its duty has already been calculated in the HP column to meet the Nitrogen purity specification. It is, therefore, specified as equal to the LP condenser duty but with a different sign to indicate that it is heating rather than cooling.

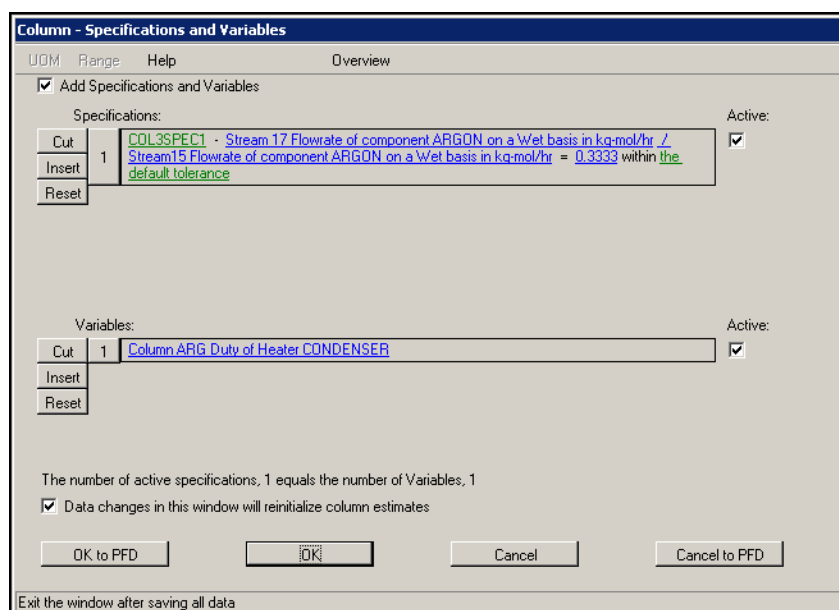
The most important specification on the LP column is the Nitrogen product purity which is set at 10 ppm Oxygen. There are two side draws which could be varied in order to meet performance specifications - the feed to the Argon column and the gaseous Oxygen product. This means that specified.

In practice, it is not a good idea to specify the Oxygen purity as this constrains the material balance very tightly. There is then a very high probability that the specifications will conflict. The best procedure is to allow the Oxygen purity to vary and fix the Argon column draw stream. The gaseous Oxygen product is then varied in order to reach solution.

Argon Column

The Argon column is modeled with a bubble point condenser and no reboiler. The vapor draw from the LP column enters the base of the column and acts as the reboiler. Because the Argon product purity is controlled by the operation of the LP column, a recovery specification is used on the Argon column. The Data Entry Window is illustrated in the following figure.

Figure: Argon Tower Specifications and Variables

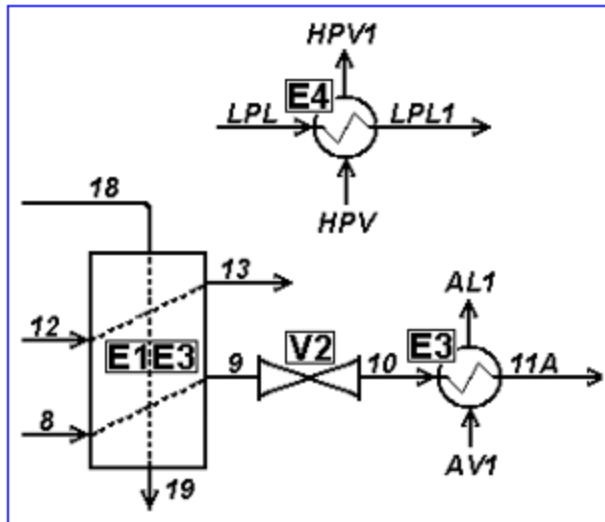


A third of the Argon in the feed is typically recovered overhead and the condenser duty can be varied in order to meet this. The expected Argon product purity is in the region of 98%. The Argon column specification is shown above. The thermodynamic method for this column is the low pressure method, 1.

Inter-Column Heat Exchanges

Once the distillation columns have solved, the exchangers between the HP and LP columns can be calculated. The following figure is a schematic of the heat exchanger simulation. Exchangers E1 and E2 (in the column section of the flowsheet) are combined into the LNGHX unit E1E2. The valves are modeled separately. Steam 18 is the Nitrogen product from the LP column, while streams 12 and 8 are the HP column products.

Figure: Inter-column Heat Exchangers



Exchangers E3 and E4 are the Argon and HP column condensers. The streams AV1 and HPV are created from the vapor flow into the condensers using the PRO/II pseudo-product stream feature. This feature models a pseudo stream that does not actually exist on the column. LPL is created from the liquid flow into the LP Column reboiler which is the other side of the HP Column condenser. These exchangers are modeled in order to enable PRO/II to check that the temperature levels are correct; i.e., there are no crossovers.

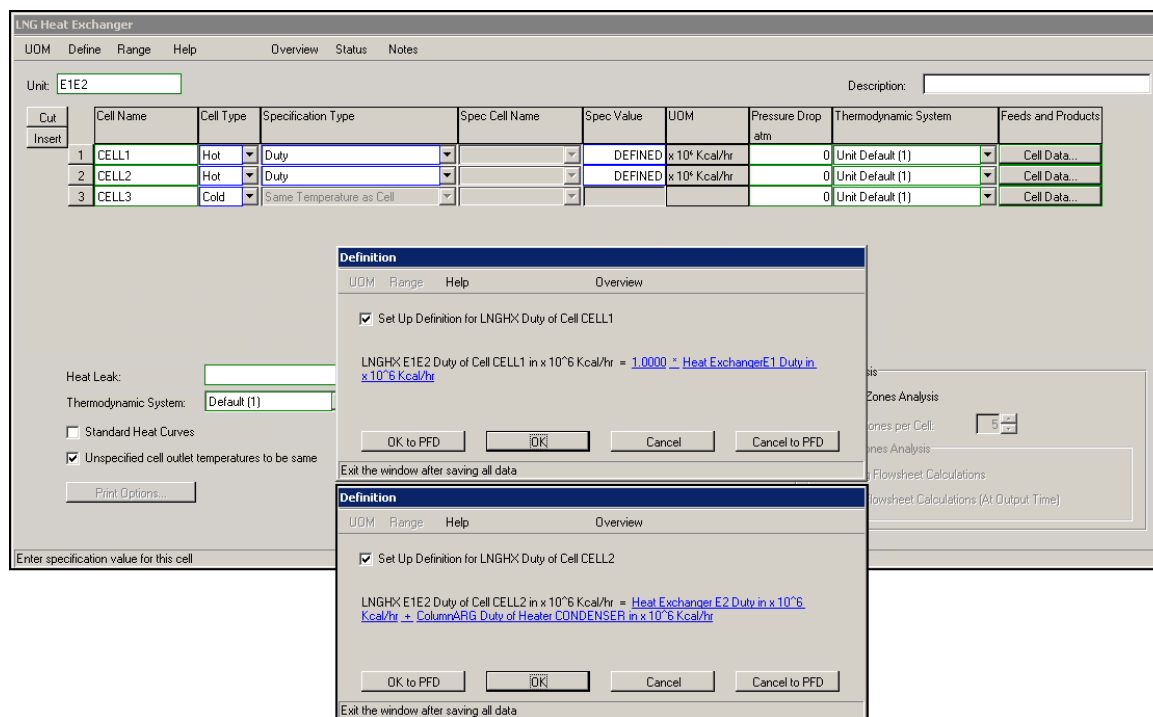
The duty on the first stream in LNG exchanger E1E2 is set equal to the duty calculated in E1 when setting the LP column feed condition. The duty on the second stream in E1E2 is defined as the duty of E2 minus the duty of the Argon column condenser. The

condenser duty is actually negative, so it is added to the E2 duty on the DEFINE statement to specify the cooling duty in E1E2.

The duties of E3 and E4 are simply defined as the same as that of the corresponding column condenser. If temperature crossovers occur, PRO/II automatically prints an error message.

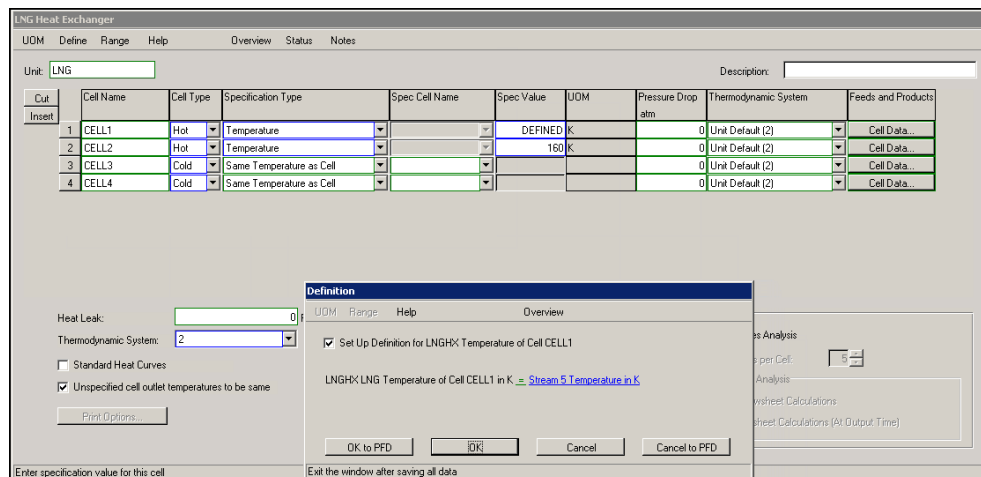
The following figure is a composite that illustrates "DEFINE-ing" duties for cells of exchanger E1E2. As the red highlights indicate, place the cursor in the DUTY field of one cell and click DEFINE on the tool bar. That action displays the Definition DEW for the selected cell.

Figure: Define DEW's for Exchanger E1E2



The following figure illustrates the DEW to DEFINE the temperature specification of cell 1 in exchanger LNG. Here the Temperature field of cell 1 is highlighted while pressing the Define button on the tool bar.

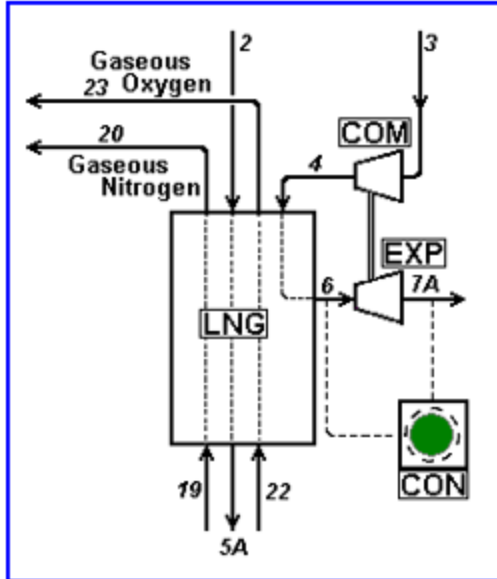
Figure: DEFINE DEW for Exchanger LNG



Heat Recovery Section

The heat recovery section consists of the LNGHX exchanger and the compressor and turbo-expander. The simulation flowsheet is shown in the following figure.

Figure: Heat Recovery Simulation Schematic

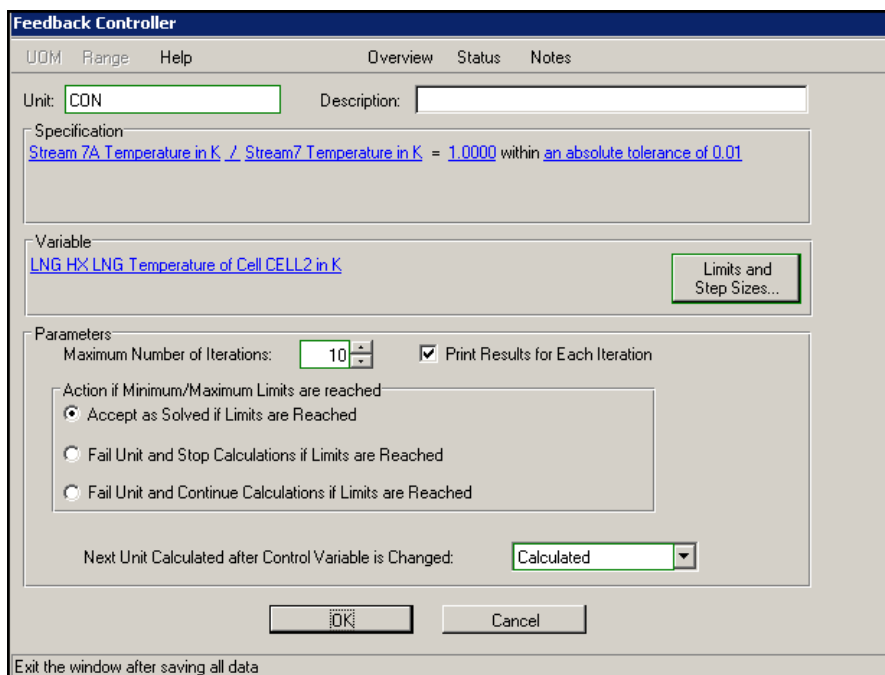


Streams 2 and 3 are the air feeds. 5A and 7A correspond to the column feed streams 5 and 7 in the column section of the flowsheet. Streams 19 and 22 are the cold gaseous Nitrogen and Oxygen products which cool the air feed.

Controller

There is an energy recycle round the three units in this section of the flowsheet and a controller is used to calculate the temperature of stream 6 leaving the LNGHX exchanger. The controller's data entry window is shown in the following figure.

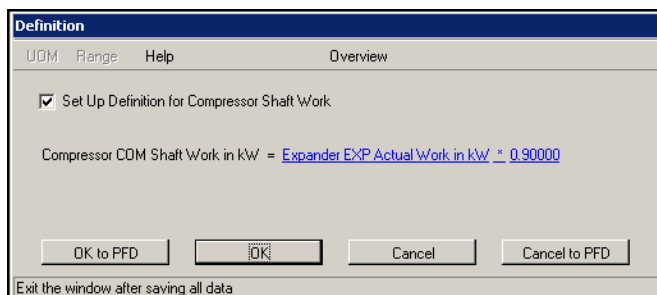
Figure: Controller Specification



Compressor/Expander

As shown in the following figure, the compressor work is defined as 90% of that produced in the expander.

Figure: Specifying Compressor Work Using DEFINE



However, when the compressor is first calculated, the expander work has not been determined. It is not possible to calculate the expander first because the inlet pressure is determined by the compressor. This means that an iterative procedure is required and it is automatically converged by PRO/II.

The temperature of stream 5A leaving the LNGHX is defined as the same as the column feed stream 5. The temperature of stream 6 is not known. However, the temperature of stream 7A leaving the expander is known. The controller is therefore used to vary the temperature of stream 6 in order to set stream 7A at the same temperature as stream 7.

Results

Column Section

The HP column solves with a condenser duty of 10.46 MKCal/hr. The overhead product is 99.83% Nitrogen with the remainder mostly Argon. The LP column reboiler duty is the same as that of the HP column condenser. The Nitrogen product contains slightly more Argon than the HP column product and is 99.72% pure. The Oxygen content is the same in both column products at the specified 10 ppm.

7.6% of the Oxygen is produced as liquid. The purity of the liquid and gas products are 99.7% and 99.6% respectively. These are both above the desired value of 99.5%.

The Argon product is 97.5% pure with 1.9% Oxygen and 0.6% Nitrogen. The product rate is 3.2% of the feed from the LP Column. The condenser duty is 2.96 MKCal/hr.

Inter-Column Exchangers

All the exchangers solve correctly which confirms that there are no temperature crossovers. The Nitrogen into the HP column condenser is at a temperature of 96.2K and the Oxygen into the LP column reboiler is at 94.8K. Because the streams are changing phase, there is very little temperature change through the exchanger.

The Argon entering the Argon column condenser is at 88.9K and is exchanging with the LP Column Oxygen product. This Oxygen stream is heated from 84.0K to 85.5K within the condenser.

The LP column Nitrogen product is heated from 79.1K to 96.3K in LNGHX unit E1E2.

Heat Recovery Section

The work recycle between the expander and compressor is solved automatically within the controller loop. The controller solves in three iterations. The compressor increases the air pressure from 6 to 9 atmospheres with an exit temperature of 320K. This is cooled in the LNGHX unit to 142K before entering the expander. It is then let down to the defined feed condition of 89.5K and 1.4 atmospheres.

APPENDIX A

Simulation Flowsheet

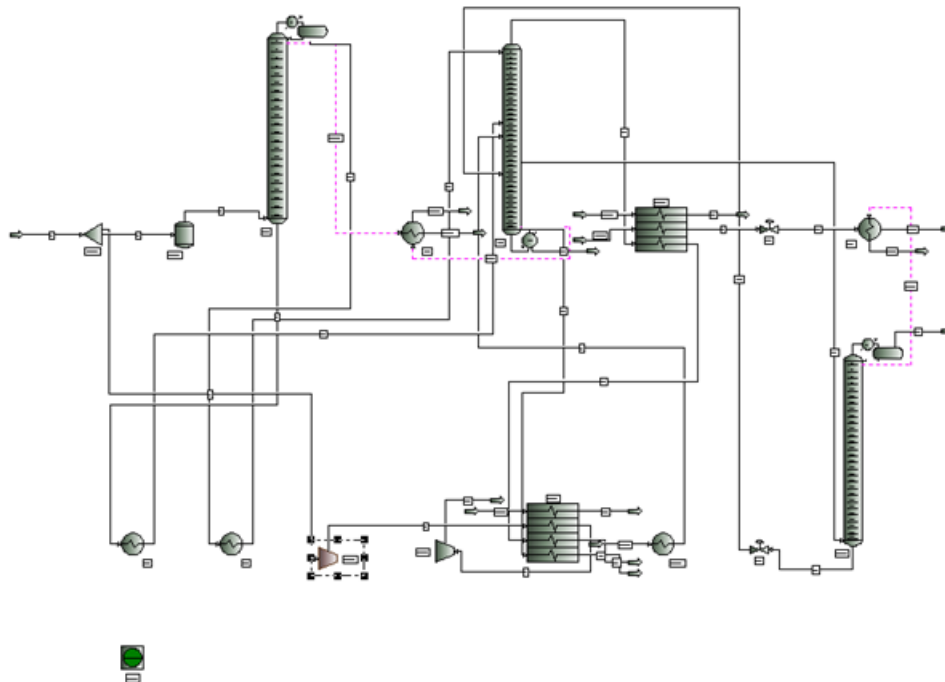
In This Appendix

PRO/II Simulation PDF	29
Column Section (Connectivity)	29
Inter-Column Heat Transfer	30

PRO/II Simulation PDF

The following figure is a representation of the complete flowsheet taken from the Piping and Flow Diagram (PFD) of PROVISION.

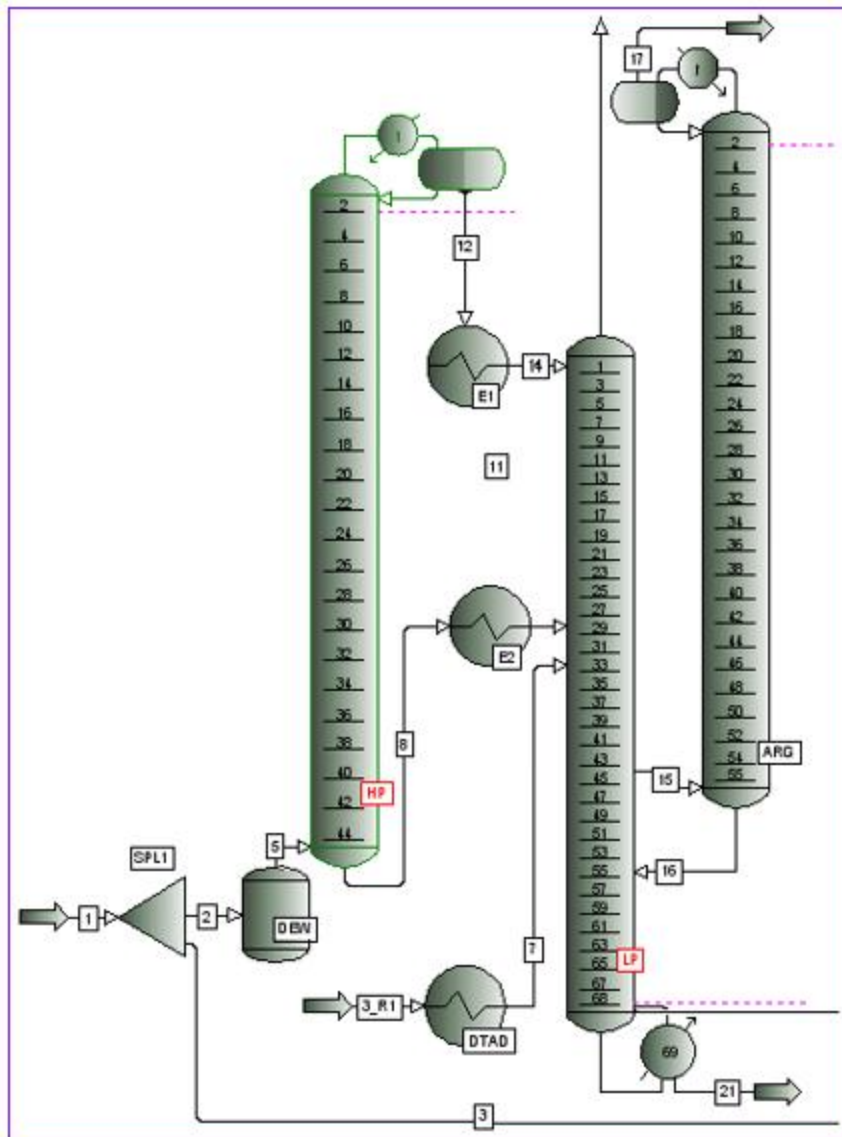
Figure: Air Separation Plant PDF



Column Section (Connectivity)

The following figure illustrates the connections of streams to the three major separation unit operations in this simulation.

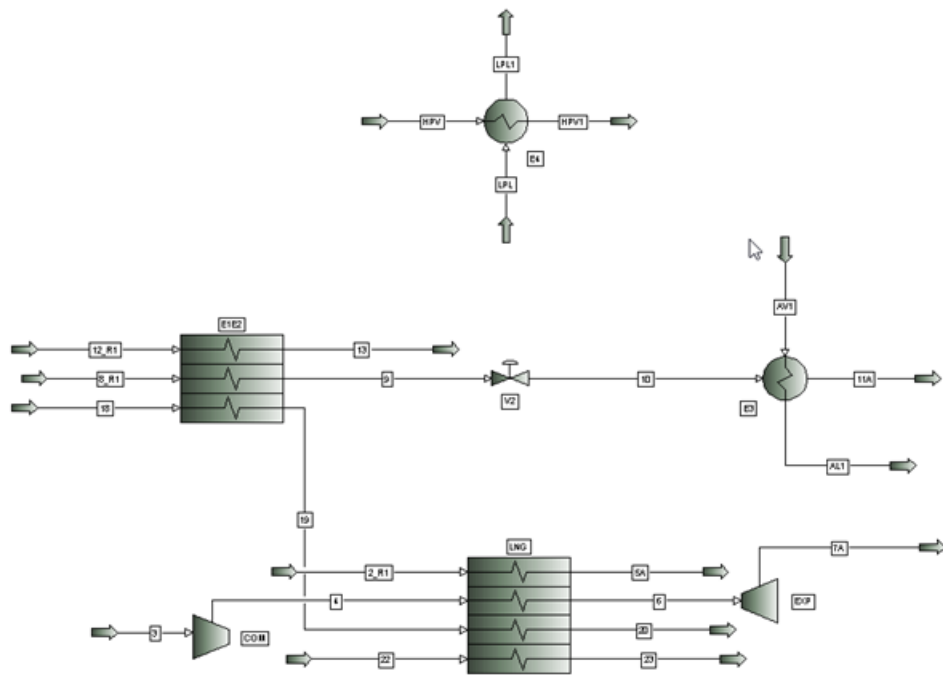
Figure: Connectivity of Distillation Units



Inter-Column Heat Transfer

The following figure shows the details of exchanging energy between streams that interconnect the major separation unit operations.

Figure: Heat Exchange Configuration Between Columns



APPENDIX B

Selected Output

The listings presented here typically are generated using the Spreadsheet tool located on the PRO/II Tools menu.

In This Appendix

Selected Stream Results	34
Compressor Results	35
Column Condensor Summary	35
HP Column Summary	36

Selected Stream Results

Figure: Selective Stream Summary

Stream Name	Description	1	18	21	22	17
Phase		AIR FEED	Vapor	O2 LIQUID	Vapor	AR PRODUCT
Total Stream Properties				Liquid		Vapor
Rate	KG-MOL/HR	9386.000	7359.621	191.989	1781.440	52.940
	KG/HR	271816.623	206506.166	6147.021	57055.198	2108.072
Std. Liquid Rate	M3/HR	311.819	255.000	5.380	49.924	1.515
Total Adj. Liq. Vol. Rate	M3/HR	804.686	655.668	14.111	130.940	3.965
Total Adj. Vap. Vol. Rate	M3/HR	210283.299	164905.838	4299.318	39892.864	1185.545
Temperature	K	278.000	78.861	94.909	94.909	88.955
Pressure	ATM	8.000	1.170	1.574	1.574	1.150
Molecular Weight		28.960	28.059	32.018	32.028	39.820
Enthalpy	M*KCAL/HR	-1.111	-11.786	-0.515	-1.885	-0.038
	KCAL/KG	-4.088	-57.073	-83.703	-33.044	-18.132
Total Liquid Fraction		0.0000	0.0000	1.0000	0.0000	0.0000
Reduced Temp.		2.1001	0.6244	0.6140	0.6140	0.5897
Pres.		0.1618	0.0348	0.0316	0.0316	0.0238
Acentric Factor		0.0341	0.0376	0.0221	0.0221	0.0004
Watson K (UOPK)		5.997	6.394	4.770	4.768	3.875
Standard Liquid Density	KG/M3	871.712	809.828	1142.526	1142.851	1391.295
Specific Gravity		0.8726	0.8106	1.1437	1.1440	1.3927
API Gravity		30.664	43.056	-7.774	-7.809	-29.896
Total Adj. Liq. Density	KG/M3	337.792	314.955	435.610	435.735	531.653
Latent Heat	KCAL/KG	n/a	n/a	n/a	n/a	n/a
Vapor Phase Properties						
Rate	KG-MOL/HR	9386.000	7359.621	n/a	1781.440	52.940
	KG/HR	271816.623	206506.166	n/a	57055.198	2108.072
Actual	M3/HR	35605.850	38908.504	n/a	8450.302	324.727
Std. Vapor Rate	M3/HR	210377.730	164958.496	n/a	39929.185	1186.593
Adj. Vap. Vol. Rate	M3/HR	210283.299	164905.838	n/a	39892.864	1185.545
Specific Gravity (Air=1.0)		1.000	0.969	n/a	1.106	1.375
Molecular Weight		28.960	28.059	n/a	32.028	39.820
Enthalpy	KCAL/KG	-4.088	-57.073	n/a	-33.044	-18.132
CP	KCAL/KG-K	0.243	0.259	n/a	0.226	0.131
Actual Density	KG/M3	7.634	5.307	n/a	6.752	6.492
Adj. Vap. Density	KG/M3	1.293	1.252	n/a	1.430	1.778
Thermal Conductivity	KCAL/HR-M-C	0.02075	0.00655	n/a	0.00721	0.00500
Viscosity	CP	0.01743	0.00552	n/a	0.00711	0.00746
Liquid Phase Properties						
Rate	KG-MOL/HR	n/a	n/a	191.989	n/a	n/a
	KG/HR	n/a	n/a	6147.021	n/a	n/a
Actual	M3/HR	n/a	n/a	5.496	n/a	n/a
Std. Liquid Rate	M3/HR	n/a	n/a	5.380	n/a	n/a
Adj. Liq. Vol. Rate	M3/HR	n/a	n/a	14.111	n/a	n/a
Specific Gravity (H2O @ 60 F)		n/a	n/a	1.1437	n/a	n/a
Molecular Weight		n/a	n/a	32.018	n/a	n/a
Enthalpy	KCAL/KG	n/a	n/a	-83.703	n/a	n/a
CP	KCAL/KG-K	n/a	n/a	0.422	n/a	n/a
Actual Density	KG/M3	n/a	n/a	1118.466	n/a	n/a
Adj. Liq. Density	KG/M3	n/a	n/a	435.610	n/a	n/a
Surface Tension	DYNE/CM	n/a	n/a	11.9875	n/a	n/a
Thermal Conductivity	KCAL/HR-M-C	n/a	n/a	0.12296	n/a	n/a
Viscosity	CP	n/a	n/a	0.17483	n/a	n/a
Solid Phase Properties						
MW Solids						
Rate	KG-MOL/HR	n/a	n/a	n/a	n/a	n/a
	KG/HR	n/a	n/a	n/a	n/a	n/a
	M3/HR	n/a	n/a	n/a	n/a	n/a
Molecular Weight		n/a	n/a	n/a	n/a	n/a
Non-MW Solids						
Rate	KG/HR	n/a	n/a	n/a	n/a	n/a
Total Solids						
Rate	KG/HR	n/a	n/a	n/a	n/a	n/a
Enthalpy	KCAL/KG	n/a	n/a	n/a	n/a	n/a
	M*KCAL/HR	n/a	n/a	n/a	n/a	n/a
CP	KCAL/KG-K	n/a	n/a	n/a	n/a	n/a
Density	KG/M3	n/a	n/a	n/a	n/a	n/a
Thermal Conductivity	KCAL/HR-M-C	n/a	n/a	n/a	n/a	n/a

Compressor Results

Figure: Report of Compressor Operations

Compressor	Name Description	COM
Compressor Data		
Outlet pressure	ATM	9.001
Pressure difference	ATM	3.001
Pressure ratio		1.500
Head fan law exponent	M	2.000
Outlet temperature	K	319.722
Specified work	KW	315.688
Head	M	4263.525
Operating RPM		N/A
Reference RPM		N/A
After cooler pressure drop	ATM	N/A
After cooler exit temperature	K	N/A
Adiabatic efficiency		82.000
Polytropic efficiency		83.005
Eff. fan law exponent		1.000
Isentropic coeff.		1.403
Polytropic coeff.		1.529
Theoretical work	KW	258.867
Polytropic work	KW	262.039
Shaft work	KW	315.692
Adiabatic work	KW	258.867
After cooler duty	M*KCAL/HR	N/A
Actual inlet vol. vapor flow	M3/HR	3560.585
Adiabatic head	M	3496.090
Polytropic head	M	3538.922
Mechanical Efficiency		100.000
Shaft Power	KW	315.692

Column Condensor Summary

Figure: Summary of Top-Tray Column Condensers

Simple Hx	Name Description		E4 HP CONDENSER	E3 CONDENSER
Hx Data				
Duty	M*KCAL/HR		10.4169	2.9775
Hot out - cold in delta T	K		1.1750	4.9301
Hot in - cold out delta T	K		1.1861	3.2593
Minimum of HOCl or HICO	K		1.1750	3.2593
Hot side product temperature	K		96.0372	88.9546
Cold side product temperature	K		94.8693	85.7078
Hot side liquid fraction			1.0000	0.9730
Cold side liquid fraction			0.0289	0.4130
Value of exchanger U*A	KCAL/HR-C		8823822.3508	737656.9490
Effective exchanger area	M2		N/A	N/A
FT factor (LMTD correction)			1.0000	0.9998
Overall exchanger LMTD	K		1.1806	4.0373
Overall exchanger LMTD from zones	K		N/A	N/A
Hotside pressure drop	ATM		0.0000	0.0000
Coldside pressure drop	ATM		0.0000	0.0000
Convergence tolerance			0.0001	0.0001
Utility inlet or satn. temp.	K		N/A	N/A
Utility saturation pressure	ATM		N/A	N/A
Utility outlet temp.	K		N/A	N/A
Utility flow rate	KG-MOL/HR		N/A	N/A

HP Column Summary

Figure: High Pressure Column Tray Operating Profile

Column HP Summary											
Tray	Temp. K	Pressure ATM	Net Flow Rates				Net Flow Rates				Duties M*KCAL/HR
			Liquid	Vapor	Feed	Product	Liquid	Vapor	Feed	Product	
			KG-MOL/HR				KG/HR				
1	96.0	5.80	5118.1			3941.7	0121.4			110528.8	-10.4169
2	96.1	5.80	5113.5	9057.8			0121.4	205761.2			
3	96.1	5.80	5111.3	9055.1			0121.4	205761.2			
4	96.1	5.81	5108.9	9052.9			0121.4	205761.2			
5	96.1	5.81	5106.3	9050.5			0121.4	205761.2			
6	96.2	5.82	5103.6	9048.0			0121.4	205761.2			
7	96.2	5.82	5100.6	9045.2			0121.4	205761.2			
8	96.2	5.82	5097.5	9042.3			0121.4	205761.2			
9	96.3	5.83	5094.1	9039.1			0121.4	205761.2			
10	96.3	5.83	5090.5	9035.8			0121.4	205761.2			
11	96.3	5.83	5088.6	9032.1			0121.4	205761.2			
12	96.4	5.84	5082.5	9028.3			0121.4	205761.2			
13	96.4	5.84	5078.0	9024.1			0121.4	205761.2			
14	96.4	5.85	5073.2	9019.7			0121.4	205761.2			
15	96.5	5.85	5068.0	9014.9			0121.4	205761.2			
16	96.5	5.85	5062.3	9009.7			0121.4	205761.2			
17	96.6	5.86	5056.2	9004.0			0121.4	205761.2			
18	96.6	5.86	5049.4	8997.8			0121.4	205761.2			
19	96.7	5.86	5041.9	8991.0			0121.4	205761.2			
20	96.8	5.87	5033.4	8983.5			0121.4	205761.2			
21	96.8	5.87	5023.9	8975.1			0121.4	205761.2			
22	96.9	5.88	5013.1	8965.6			0121.4	205761.2			
23	97.0	5.88	5000.8	8954.8			0121.4	205761.2			
24	97.1	5.88	4988.7	8942.4			0121.4	205761.2			
25	97.2	5.89	4970.5	8928.3			0121.4	205761.2			
26	97.3	5.89	4952.1	8912.2			0121.4	205761.2			
27	97.4	5.90	4931.0	8893.7			0121.4	205761.2			
28	97.6	5.90	4907.3	8872.7			0121.4	205761.2			
29	97.8	5.90	4880.7	8848.9			0121.4	205761.2			
30	97.9	5.91	4851.5	8822.4			0121.4	205761.2			
31	98.2	5.91	4820.0	8793.2			0121.4	205761.2			
32	98.4	5.91	4788.6	8761.6			0121.4	205761.2			
33	98.6	5.92	4752.2	8728.3			0121.4	205761.2			
34	98.9	5.92	4717.6	8693.9			0121.4	205761.2			
35	99.1	5.93	4683.8	8659.3			0121.4	205761.2			
36	99.4	5.93	4651.8	8625.5			0121.4	205761.2			
37	99.6	5.93	4622.1	8593.4			0121.4	205761.2			
38	99.8	5.94	4595.5	8563.8			0121.4	205761.2			
39	100.0	5.94	4572.2	8537.2			0121.4	205761.2			
40	100.2	5.94	4552.2	8513.9			0121.4	205761.2			
41	100.4	5.95	4535.5	8493.9			0121.4	205761.2			
42	100.5	5.95	4521.7	8477.1			0121.4	205761.2			
43	100.6	5.96	4510.5	8463.3			0121.4	205761.2			
44	100.7	5.96	4505.7	8452.1	8447.4	4505.7	0121.4	205761.2	244634.9	134106.2	

Figure: High Pressure (HP) Column Composition Profile

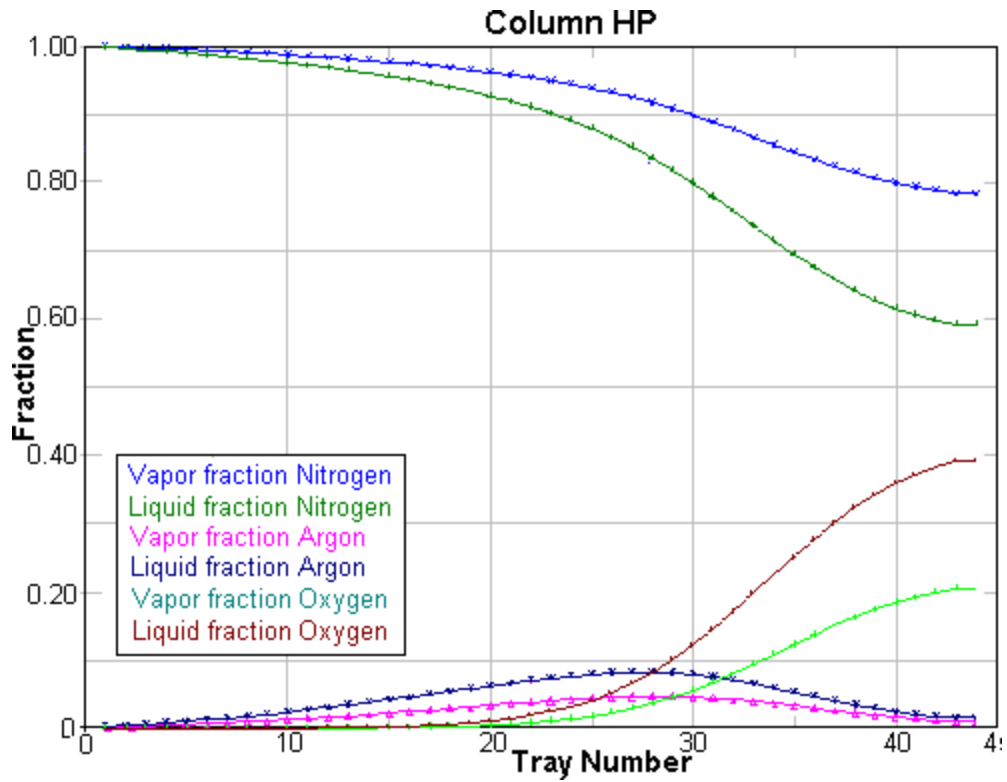


Figure: Low Pressure (LP) Column Feeds and Products

Column LP Streams & Duties			
Tray	Feed	Product	Duties
	KG-MOL/HR.		
1	3943.2	7359.7	
28	4504.2		
32	938.6		
44		1875.0	
45	1821.5		
69		1972.7	10.4164

Figure: Low Pressure (LP) Column Composition Profile

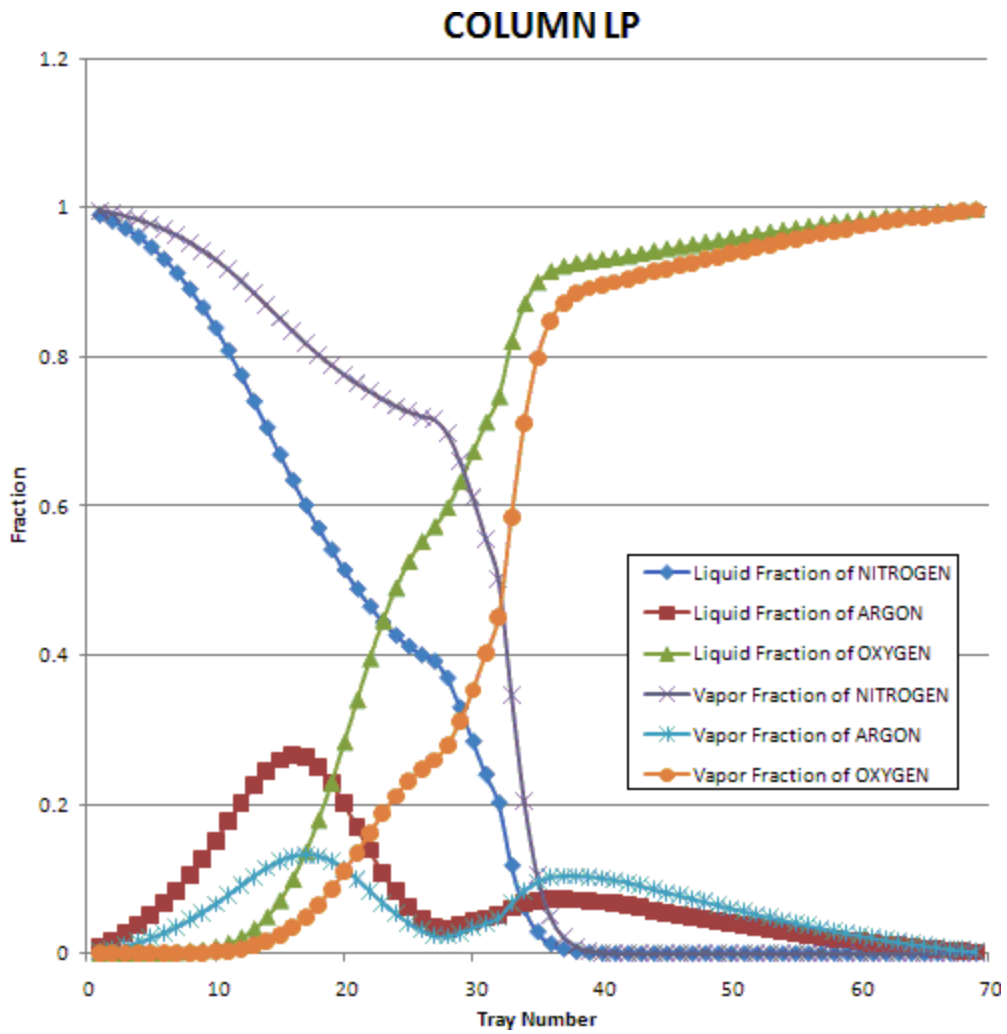
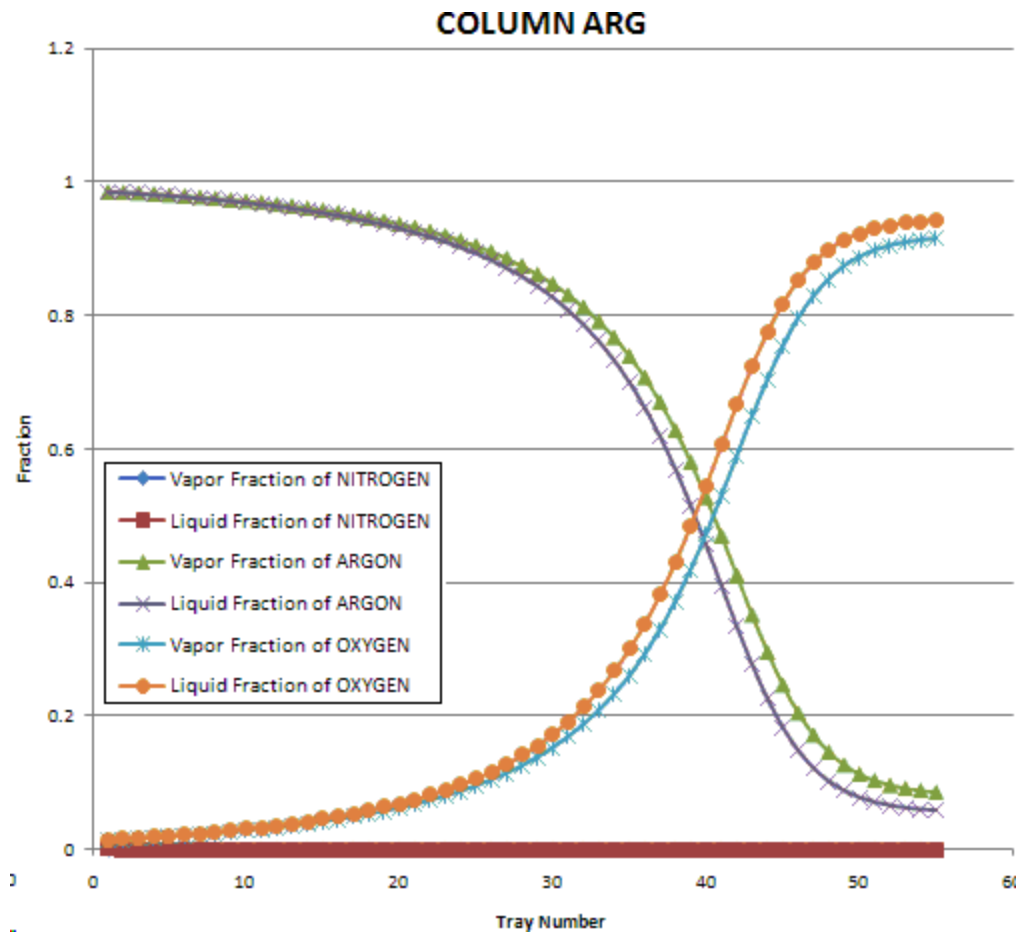


Figure: Argon Column Composition Profile



APPENDIX C

Keyword Input File

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$ Generated by PRO/II Keyword Generation System <version 10.2>
$ Generated on: Thu Aug 09 09:58:30 2018
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  PRINT INPUT=ALL, STREAM=COMPONENT, RATE=M, FRACTION=M, MBALANCE=ON, &
    HISTORY=ON
  TOLERANCE STREAM =0.001,-0.00555555555555556,1e-005,0.01, &
    TEMPERATURE=-0.00055555555555556, PRESSURE=0.001, &
    DUTY=0.0001, MISCELLANEOUS=0.001, FLASH=3e-006, MBAL=1
  DIMENSION METRIC, MDUTY=ON, BASIS=MOLE, TEMP=K, PRES=ATM, WT=KG, &
    TIME=HR, LENGTH=M, FLENGTH=MM, LIQVOL=M3, VAPVOL=M3, &
    LDENSITY=KG/M3, VDENSITY=KG/M3, XDENSITY=DENS, &
    SPVOL=M3/KG-MOL, SPVVOL=M3/KG-MOL, ENERGY=KCAL, WORK=KW, &
    DUTY=KCAL/HR, CONDUCT=KC/H, HTCOCF=KC/H, FOUL=HMC/K, &
    VISCOSITY=CP, KVIS=CST, SURFACE=D/CM, STDTEMP(C)=0, &
    STDPRES (KG/CM2)=1.0332274528, PBASIS (KG/CM2)=1.0332274528
  SEQUENCE SIMSCI
  CALCULATION TRIALS=50, RECYCLE=ALL, TVPBASIS=310.9277777778, &
    RVPBASIS=APIN, COMPCHECK=CALC, MAXOPS=1000000, CDATA=FIX, &
    FLASH=DEFAULT, DVARIABLE=ON, PHASE=SIMSCI, TMAX=OLDLIMIT, &
    TMIN=OLDLIMIT
COMPONENT DATA
  CURRENT SEARCH = SIMSCI,PROCESS
  LIBID 1,NITROGEN/2,ARGON/3,OXYGEN, BANK=CURRENT
THERMODYNAMIC DATA
  TRESET CONSTANT = NOFLASH
  METHOD SYSTEM=SRK, DENSITY(L)=IDEAL, SET=1, DEFAULT
  WATER PROPERTY=IF97, TRANSPORT=IF97
  KVAL(VLE)
    SRK 1,3,-0.00694,0,0,0
    SRK 1,2,0.0056,0,0,0
    SRK 2,3,0.01574,0,0,0
  METHOD SYSTEM=SRK, DENSITY(L)=IDEAL, SET=2
  WATER PROPERTY=IF97, TRANSPORT=IF97
  KVAL(VLE)
    SRK 1,3,-0.01089,0,0,0
    SRK 1,2,0,0,0,0
    SRK 2,3,0.01697,0,0,0
STREAM DATA
  PROPERTY STREAM=1, TEMPERATURE=278, PRESSURE=6, PHASE=M, &
    RATE (M)=9386, COMPOSITION (M)=1,78.11/2,0.93/3,20.96
  PROPERTY STREAM=16, TEMPERATURE=92.79, PRESSURE=1.32, PHASE=L, &
    COMPOSITION (M,KGM/H)=2,104.63/1,0.0372725/3,1717.23
  PROPERTY STREAM=8_R1, REFSTREAM=8
  PROPERTY STREAM=12_R1, REFSTREAM=12
  PROPERTY STREAM=3_R1, REFSTREAM=3
  PROPERTY STREAM=2_R1, REFSTREAM=2
  NAME 1,AIR FEED/16,ARG BTMS/8,HP BTMS/12,HP OVHD/15,ARG FEED/ &
    17,AR PRODUCT/20,N2 PRODUCT/23,O2 GAS/21,O2 LIQUID
UNIT OPERATIONS
  SPLITTER UID=SPL1, NAME=FEED SPLIT

```

```

FEED 1
PRODUCT M=2, M=3
OPERATION OPTION=FULL
SPEC STREAM=3, RATE (KGM/H), TOTAL, WET, DIVIDE, STREAM=1, &
      RATE (KGM/H), TOTAL, WET, VALUE=0.1
METHOD SET=2
FLASH UID=DEW
FEED 2
PRODUCT V=5
DEW DP=0
COLUMN UID=HP, NAME=HP COLUMN
PARAMETER TRAY=44, IO
FEED 5, 44, TNOTSEPARATE, NOTSEPARATE
PRODUCT OVHD (M)=12, 4000, BTMS (M)=8, SUPERSEDE=ON
CONDENSER TYPE=BUBB
DUTY 1, 1, , CONDENSER
PSPEC PTOP=5.8, DPCOLUMN=0.16
PRINT PROPTABLE=PART
ESTIMATE MODEL=CONVENTIONAL, REFLUX=5500
SPEC ID=COL1SPEC1, STREAM=12, PPM, COMP=3, WET, VALUE=10
VARY DNAME=CONDENSER
TFLOW NET (V)=HPV, 2
METHOD SET=2
HX UID=E1
HOT FEED=12, M=14, DP=4.6
OPER HLFAC=0.9
HX UID=E2
HOT FEED=8, M=11, DP=4.55
OPER HLFAC=0.45
HX UID=DTAD
HOT FEED=3_R1, M=7, DP=4.6
OPER HDTADEW=5
VALVE UID=V1
FEED 16
PRODUCT M=S1
OPERATION PRESSURE=1.4433
COLUMN UID=LP, NAME=LP COLUMN
PARAMETER TRAY=69, IO
FEED 14, 1, TNOTSEPARATE/11, 28, TNOTSEPARATE/7, 33, TNOTSEPARATE/ &
      S1, 47, TNOTSEPARATE, NOTSEPARATE
PRODUCT OVHD (M)=18, 7800, VDRAW (M)=22, 69, 1800, VDRAW (M)=15, 44, &
      1875, BTMS (M)=21, SUPERSEDE=ON
DUTY 1, 69, 8, SIDEHC1
PSPEC PTOP=1.17, DPCOLUMN=0.404
PRINT PROPTABLE=PART
ESTIMATE MODEL=CONVENTIONAL, REFLUX=3500
SPEC ID=COL2SPEC1, DNAME (MMON, KC/H)=SIDEHC1, DIVIDE, COLUMN=HP, &
      DNAME (MMON, KC/H)=CONDENSER, VALUE=-1
SPEC ID=COL2SPEC2, STREAM=18, PPM, COMP=3, WET, VALUE=10
VARY DNAME=SIDEHC1
VARY DRAW=22
PLOT PROFILE, XCOMPONENT=1, 1/2, 2/3, 3, YCOMPONENT=1, 1/2, 2/3, 3
TFLOW NET (L)=LPL, 68
METHOD SET=1
COLUMN UID=ARG, NAME=ARGON COLUMN
PARAMETER TRAY=55, IO
FEED 15, 55, TNOTSEPARATE, NOTSEPARATE
PRODUCT OVHD (M)=17, 100, BTMS (M)=16, SUPERSEDE=ON

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CONDENSER TYPE=PART
DUTY 1,1,-3,CONDENSER
PSPEC PTOP=1.15, DPCOLUMN=0.17
PRINT PROPTABLE=BRIEF
ESTIMATE MODEL=CONVENTIONAL, REFLUX=1500
SPEC ID=COL3SPEC1, STREAM=17, RATE (KGM/H), COMP=2,WET, DIVIDE, &
      STREAM=15, RATE (KGM/H), COMP=2,WET, VALUE=0.3333
VARY DNAME=CONDENSER
TFLOW NET (V)=AV1,2
METHOD SET=1
LNGHX UID=E1E2
  HOT FEED=12_R1, M=13, NUMBER=1, CELL=CELL1
  HOT FEED=8_R1, M=9, NUMBER=2, CELL=CELL2
  COLD FEED=18, M=19, NUMBER=3, CELL=CELL3
  OPER TSAME=YES
  DEFINE DUTY (1,MMON,KC/H) AS 1, TIMES, HX=E1, DUTY (MMON,KC/H)
  DEFINE DUTY (2,MMON,KC/H) AS HX=E2, DUTY (MMON,KC/H), PLUS, &
      COLUMN=ARG, DNAME (MMON,KC/H)=CONDENSER
COMPRESSOR UID=COM
  FEED 3
  PRODUCT V=4
  OPERATION CALCULATION=GPSA, COPT=SING, EFF=82
  DEFINE WORK (KW) AS EXPANDER=EXP, WORK (KW), TIMES,0.9
  METHOD SET=2
LNGHX UID=LNG
  HOT FEED=2_R1, M=5A, NUMBER=1, CELL=CELL1
  HOT FEED=4, M=6, TEMP=160, NUMBER=2, CELL=CELL2
  COLD FEED=19, V=20, NUMBER=3, CELL=CELL3
  COLD FEED=22, V=23, NUMBER=4, CELL=CELL4
  OPER TSAME=YES
  DEFINE TEMP (1,K) AS STREAM=5, TEMPERATURE (K)
  METHOD SET=2
EXPANDER UID=EXP
  FEED 6
  PRODUCT V=7A
  OPERATION PRES=1.4, EFF=85
CONTROLLER UID=CON
  SPEC STREAM=7A, TEMPERATURE (K), DIVIDE, STREAM=7, &
      TEMPERATURE (K), VALUE=1, ATOLER=0.01
  VARY LNGHX=LNG, TEMP (2,K)
  CPARAMETER IPRINT, SOLVE
VALVE UID=V2
  FEED 9
  PRODUCT M=10
  OPERATION DP=4.55
HX UID=E3, NAME=AR CONDENSER, ZONES (OUTPUT)=5
  HOT FEED=AV1, L=AL1
  COLD FEED=10, M=11A
  CONFIGURE COUNTER
  DEFINE DUTY (MMON,KC/H) AS -1, TIMES, COLUMN=ARG, &
      DNAME (MMON,KC/H)=CONDENSER
HX UID=E4, NAME=HP CONDENSER, ZONES (OUTPUT)=5
  HOT FEED=HPV, L=HPV1
  COLD FEED=LPL, M=LPL1
  CONFIGURE COUNTER
  DEFINE DUTY (MMON,KC/H) AS -1, TIMES, COLUMN=HP, &
      DNAME (MMON,KC/H)=CONDENSER
END

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