Air Separation Units (ASUs) Simulation Using Aspen Hysys® at Oxinor I of Air Liquid Chile S.A Plant

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The method used to extract copper from its ores depends on the nature of the ore. The main process currently to separate copper from sulphide ores is the smelting process. The concentrated ore is heated strongly with silicon dioxide (silica), calcium carbonate and oxygen enriched air in a furnace or series of furnaces which is carried out using the injection of the air for oxidation the Fe and Si present in the raw material. Oxygen can be produced using several different methods. One of these methods is Air separation process, which separates atmospheric air into its primary components, typically nitrogen and oxygen, and sometimes also argon and other rare inert gases by cryogenic distillation. In this paper, simulation of air separation units (ASUs) was studied using Aspen Hysys®. The obtained simulation and model was validated with the operational data from the Oxinor I of Air Liquide S.A Plant. The ASU was divided into subsystems to perform the simulations. Each subsystem was validated separately and later on integrated into a single simulation. An absolute error of 1% and 1.5% was achieved between the simulated and observed the process variables(s). This indicated that Aspen Hysys® has the thermodynamic packages and required tools to perform simulations in cryogenic processes at industrial scale.

Keywords: Simulation, Oxygen plant, Aspen Hysys, Air separation units (ASUs), Air Liquide S.A.

INTRODUCTION

The main process to separate copper sulphides from ferrous metals is the copper smelting process, which is carried out by injecting pure oxygen into the minerals in order to oxidize the Fe and Si present in the raw material. Only in Chile between 2010 and 2016, 14531.8 kMT of ore were processed at the smelter plants[1]. Taking into account that each ton of material requires 42 m³ of Oxygen, it can be seen that the need for this supply is of high value for foundry companies.

Due to the importance of the oxygen supply in copper sulphide treatment plants, an emphasis is needed on the production of this raw material. Obtaining O_2 is performed in several ways, some of them are absorption of gases using zeolite or other synthetics materials, chemicals reactions and the cryogenic process, the main one being a unit called ASU (Air Separation Unit) because of its capability to produce large volumes of high purity products, it uses cryogenic processes to obtain pure oxygen in liquid or in its gaseous form[2]

There has been investigation to optimize the processes of an ASU with the purpose of determining its use in power generation systems[3]. The complexity of the cryogenic processes, due to its low temperatures, makes the simulation process difficult, which is why simulation software is used to help with this task. The software that has been used and tested by different researchers is Aspen Hysys®[4]. Other software used in this area is gProm[5].

Different approaches have been taken to simulation of oxygen plants and their energy efficiency. Studies have been carried out emphasizing the separation process by modifying variables or stages of the process[6]. Others have performed simulations in complete plants, optimizing electricity consumption and Oxygen production[7].

Many researchers have used the Aspen Hysys tool to simulate power generation plants through integrated gas cycles, within which ASU systems are an essential part of the process[8]. Up to now the published work focused on qualitative changes in the gas processes for energy production[9]. Other investigations have been carried out simulations in specific equipment such as cryogenic distillation columns or pumps of subcooled fluids[10] some researchers have used Aspen Hysys to simulate cryogenic CO_2 removal plants[11].

In this paper, simulation of air separation units (ASUs) was studied using Aspen Hysys®. The obtained simulation and model was validated with the operational data from the Oxinor I of Air Liquide S.A Plant. The aim of this work is to provide Airliquide Chile S.A. a validated tool to simulate the operation variables for the purpose of process optimization.

Air separation process

The Cryogenic Air separation process involves several main and a few secondary stages. First, the air must be filtered so that impurities such as dust or other contaminants are eliminated. Once the air is filtered the process begins with the gas compression. For this, the fluid must pass through a three-stage turbocharger. Tube & Shell heat exchangers are then used to make the compression adiabatic.

After compression the washing stage begins, which is to clean the air from contaminants that may exist, such as carbon dioxide and water vapor this is done by cooling the compress air with cool water in a washing tower then the humid air pass through a fixed bed column that adsorb the CO_2 and water vapour. After cleaning the gases, the stream is separated into two streams, one of them, which we call MP (medium pressure), goes directly to the next stage called cold box, the rest of the fluid goes through a second compression, which increases the gas pressure using a two-stage turbocharger and a tube

& shell heat exchanger. The resulting stream, called HP (High Pressure), enters the cold box stage.

In the cold box stage we have the heart of all ASU processes which consist of several items of equipment such as heat exchangers, vaporizers, pumps and the distillation columns, both HP and MP.

Figure 1 shows a block diagram exemplifying the process of an ASU. There are two distillation columns one working at high pressure(HP) and one working at medium pressure(MP), in the HP column the air is separated into a stream of pure nitrogen at the top and at the bottom an impure oxygen stream, the MP column has the purpose of purify the O_2 stream.

SOFTWARE AND METHODS

Software

As software, the Aspen Hysys® Software acquired by the Universidad Católica del Norte, Antofagasta Chile, as shown in the Figure 2 , was used to carry out the simu-

lations. Aspen Hysys® developed by Aspen Technology has a library of more than ten thousand components added to a library of thermodynamic equations that includes more than ten equations of state each with their corresponding models and parameters. Specializes in steady-state analysis. The validations were performed using the data obtained from the Oxinor I operation from Air Liquide S.A. As a thermodynamic package, the Equilibrium model from Peng-Robinson modified by Stryjek and Vera[12] was used.

Methodology

As a methodology, it was decided to address the problem of the simulation of an ASU plant in the form of its internal operations by dividing the plant into the following subsystems. This decision was made because the processes and operations that involve an ASU are so complex that to try a unique simulation where it involves the whole process would be chaotic and could not be appreciated in detail the errors and deviations in
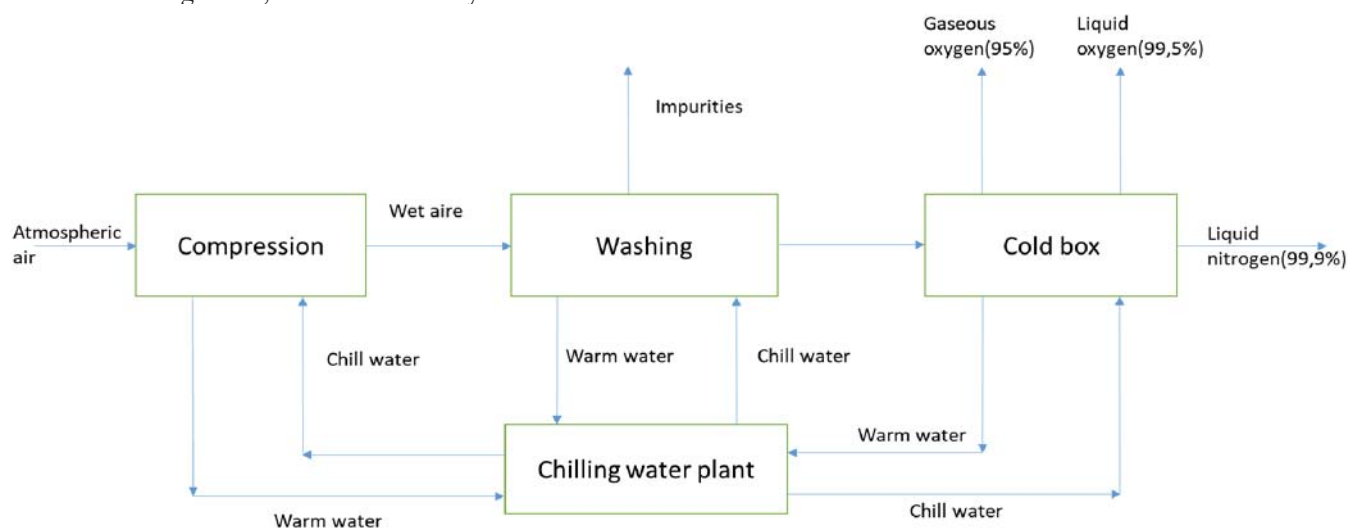

Figure 1. A block diagram of demonstrating the ASU process
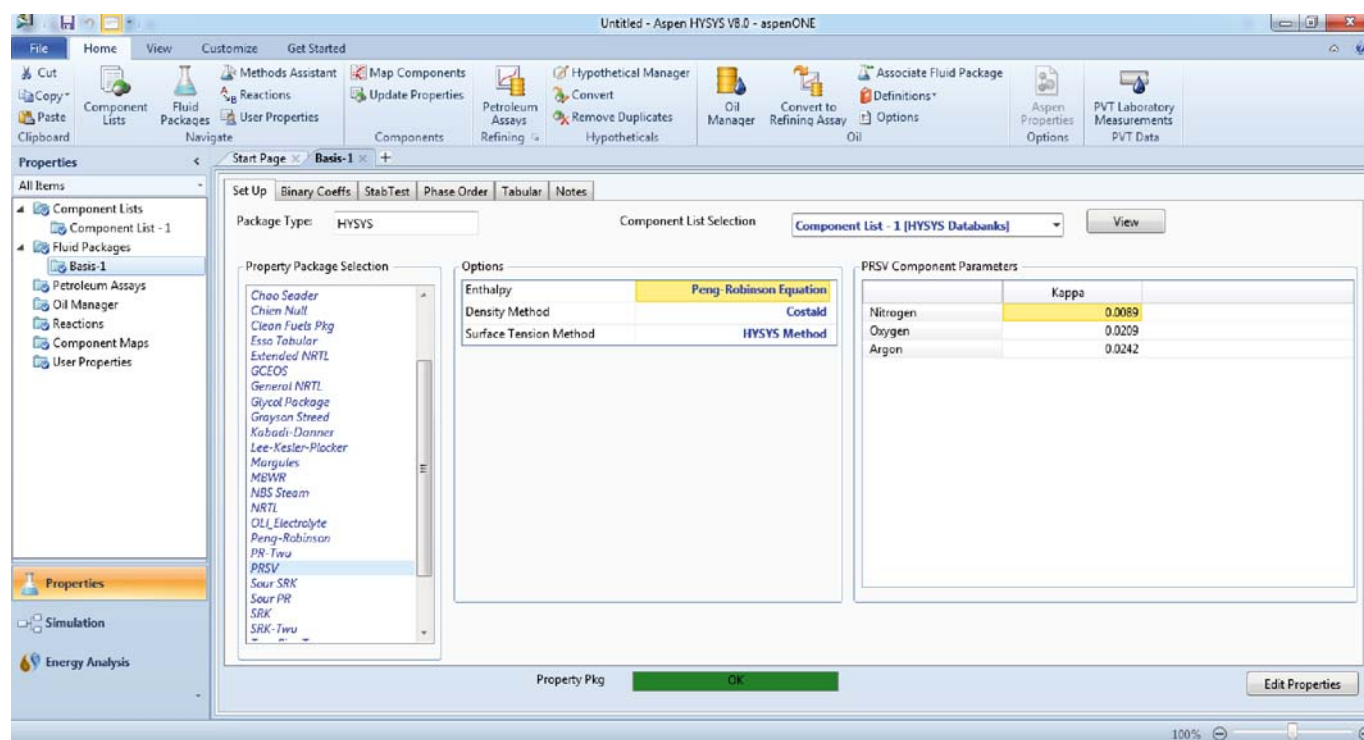

Figure 2. Aspen Hysys® owned by the Universidad Católica del Norte

the variables of process. If they are simulated separately you can ensure that each stage works on its own and then simulate the entire process in one step:
- Compression;
- Washed;
- Cold box; and
- Water cooling plant.

These divisions were validated independently with operational data. Once the parts were simulated and validated we proceeded to join the stages to form the process. The plant was validated with the same data.

Stages

Compression

The compression consisted of two separate phases, a primary compression performed by a three-stage turbo compressor and a secondary compression performed by a two-stage turbo compressor. The first compression occurs at the introduction of the atmospheric air and the second compression after adsorption stage.

Primary compression

This first compression consists of a three-stage turbo compressor already mentioned, after each stage there are tube and shell heat exchangers that cool the air coming out of the compression sections in counter flow with water. The purpose of this stage is to raise the atmospheric air pressure to the working pressures of the cryogenic distillation zones. There is a filter at the opening of the compressor to prevent the ingress of particulate material.

Secondary compression

The second compression uses two compression stages and a shell and tube heat exchanger to compress and cool a portion of the air from the washing step in order to achieve the pressure required to operate the distillation columns.

Washing step

This stage consists of two main parts, which are gas cooling and an adsorption of impurities. The removal of water and CO_2 present as impurity is carried out in adsorption columns. The gases are cooled by backwashing in direct contact with cold water.

Cold Box

The process of the cold box has the purpose of producing products desired by the needs of the market. This stage consists of plate heat exchangers, HP and LP distillation towers, auxiliary vaporizers, and a booster / turbine system.

Booster /turbine system

The compressor/turbine is equipment that provides the cooling required for the separation of air to occur. The compressor compresses the air and later in the turbine, the air is expanded causing it to cool and thus resulting in the normal operating conditions necessary to compensate for the cold losses of the system and to provide the cooling power for the generation of liquid products. The equipment has a tube and shell heat exchanger.

Water cooling plant

As mentioned above, the tube and shell heat exchangers use water to cool the various gases, this is why the Oxinor I plant has two water circulation systems called Closed and Open Circuit. Both circuits are connected by plate heat exchangers.

The open circuit consists of a cooling tower, a pump and the plate exchanger. The cooling tower is a device that uses atmospheric air to cool the water by direct contact and uses a fan system to circulate the air through the water, which is cooled by saturation of the air. The purpose of this system is to cool the water that can be used in the wash tower.

The closed circuit is composed of a pump, a plate heat exchanger and an accumulator. This circuit is intended to provide cooling water to the heat exchangers during the compression stages. Each circuit has two A and B connections, which are two different heat exchangers.

Validation methodology

For the verification of the compression stages, it was decided to adjust the adiabatic efficiencies of each step and the heat transfer coefficients of the heat exchangers. As input variables, the value of temperature, pressure and flow sensors from the plant were taken into the input of each compression and cooling step. The temperatures and pressures were compared to the output of each equipment.

For the washing step, it was decided that the best way to adjust the simulation to the plant data would be to calculate the pressure losses in both the cooling column and the adsorber, in addition the pump design data was used to obtain the characteristics curves of the pumps. The pressures obtained with the plant data were compared in the cooling columns, adsorber and centrifugal pumps.

For the validation of the turbine compressor system, the adiabatic efficiencies of both the compressor and the turbine and the heat transfer coefficient of the heat exchanger were used, the output values were used to compare the simulation results with the plant data.

Based on the information that was obtained from the cold box, it was decided to maintain certain temperatures, that are constant in the process, and to modify the inflow and production flows of the distillation columns in order to be able to compare the quality of gaseous oxygen upon exit.

For the validation of the water cooling plant it was decided to determine the outlet temperatures of the plate exchangers depending on the input temperatures of both closed and open circuits. For the cooling tower of air, the temperature at exit was found to be a function of the one at entrance.

RESULTS

Compression results

From the results of the compression the temperatures obtained by the simulator and the temperatures of the plant sensors were analyzed (T1: input to second compression stage and T2: outlet of compression stage). The flowsheet used to simulate this stage is shown on
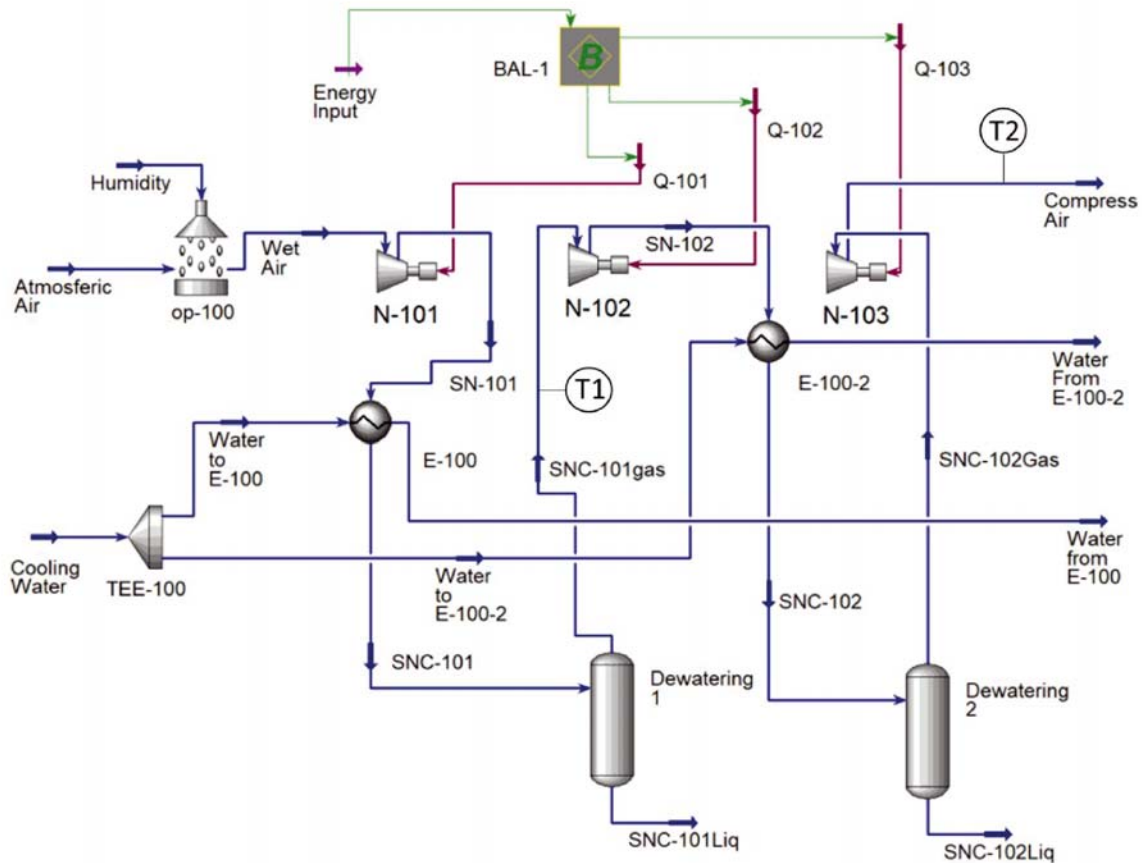
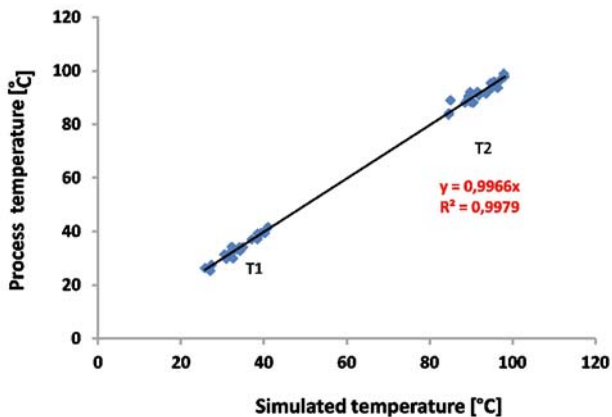**Figure 3.** Compression stage simulation flow sheet

Figure 4. Linear regression of compression stage

Figure 3. A linear regression was made to the data to see the difference in the simulated and the real values. The results are plotted in Figure 4. A regression index of 0.9979 was obtained. As it can be seen in the Figure 4 the data simulated a high concordance with the data from the plant sensors.

Washing stage results

From the washing step, the outlet pressures of the absorption and wash towers were taken and compared with the data from the plant sensors. The simulation flowsheet used to run the programs is show on Figure 5. The results are shown in Figure 6. A regression index of 0.9648 was obtained (P1). If we look close in the Figure 6 it can be seen that the data obtain from the simulator and the plant data has a high similarity however it can still be improve changing some parameters. As Aspen

Hysys® doesn't have an air/solid separation module a component splitter was used instead, separating the air stream and it is component (N_2, O_2 and Argon) of the impurities such as CO_2 and water vapor.

For pressures losses the following equations were obtained:

Column N114

$$P_{ouput} = 0,85 * P_{input} + Air\ Flow_{input} * 5,79 * 10^{-6} + 47,60 \qquad (1)$$

Adsorber N18

$$P_{ouput} = 0,96 * P_{input} + Air\ Flow_{input} * 1,74 * 10^{-9} + 7,180 \qquad (2)$$

Pump N113

$$H = -6,017 * Q^2 + 3,6979 * Q + 55,77 \qquad (3)$$

Pump N115

$$H = -133,7 * Q^2 + 29,886 * Q + 97,639 \qquad (4)$$

Where:
P_{output} – Ouput pressure [Kpa]
P_{input} – Input pressure [Kpa]
Air flow – Input air flow in each equipment [Nm^3/h]
H – Head [m]
Q – Water flow [m^3/h]

Cold box

In the cold box stage, shown on Figure 7, the results of the O_2 flow (F1) were obtained at the exit of this stage and de temperature inlet to the plate exchange. The plant data were used to validate the obtained data. The results were plotted Figure 8 (F1 and T3). Regression indices 0.9475 and 0.8782 respectively were obtained. Figure 8 shows a lower regression index, but taking into account the complexity and quantity of equipment and
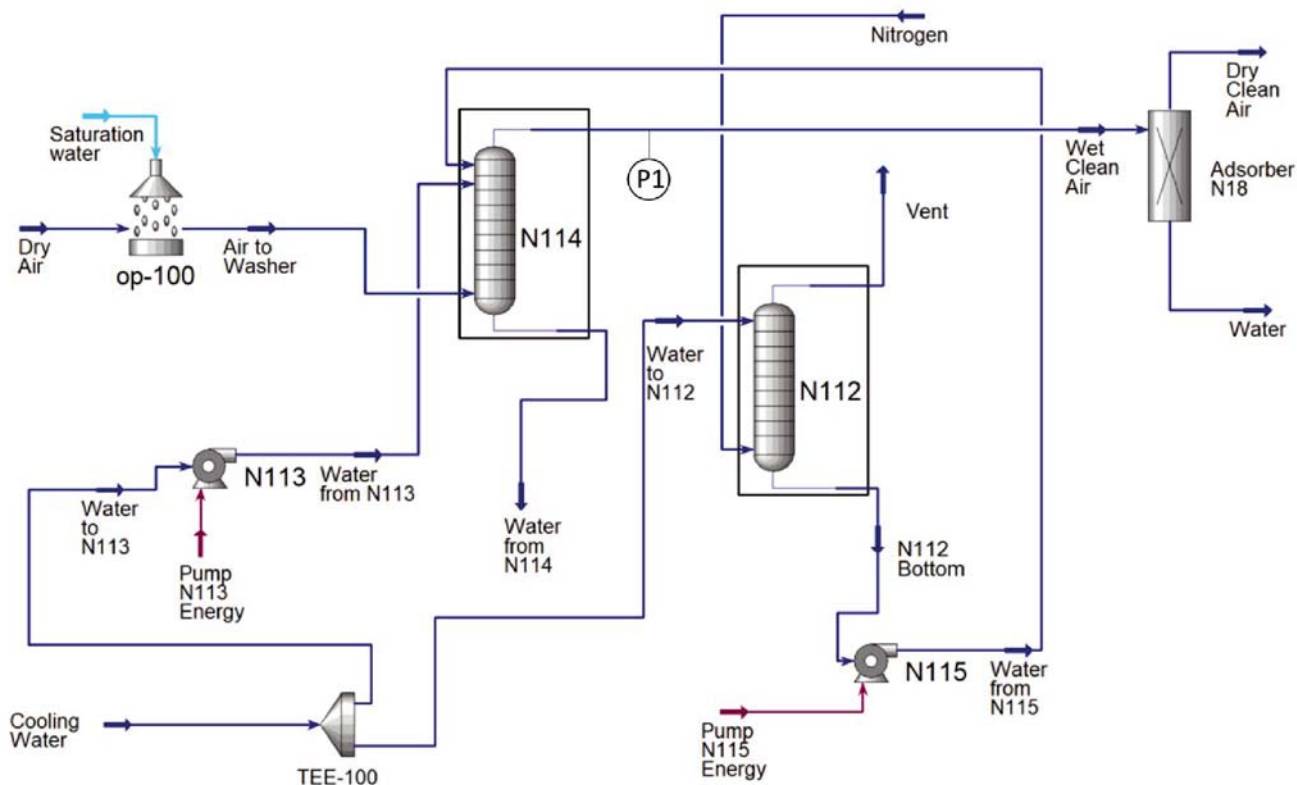
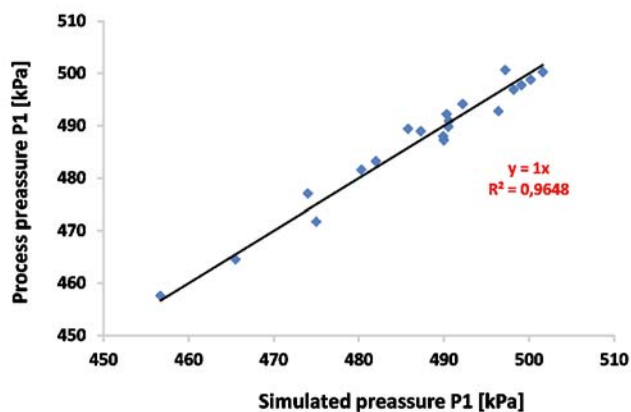**Figure 5.** Washing stage simulation flow sheet

Figure 6. Linear regression of washing stage

flows within the system it can be said that the index is sufficiently valid to consider this stage validated with the simulation data in contrast to the values Plant

Water Cooling plant

For the water plant, we took the data from two circuits plant A and B. The output temperatures of closed circuits A, closed B, open A and open B were simulated (T4, T5, T6 and T7). The simulation flow sheet is shown on Figure 9. The results are plotted in Figure 10. It can be observed that circuit A has a higher regression index than circuit B. This can be due to many reasons, such as a discrepancy of data in the sensors of both circuits, the difference in the maintenance of both circuits, and the use that is given to each system.

Error analysis

In order to establish the errors in the different validations, a variance analysis was performed on the absolute errors of the studied and validated variables, finding with

a certainty of 95% that the error is between 1% and 1.5% comparing the value delivered by the simulator and the value of the sensor. The error distribution chart is shown on the Figure 11.

DISCUSSIONS

Observing the results of the simulated stages of the process, we can see that the regression coefficients are mostly between 0.9 and 0.95, which allows us to concisely state that the values used in the simulation are in line with the reality of the plant allowing achievement of outputs near the process values.

Certain stages such as the cold box, specifically the flow of O_2 must be looked at more extensively since its regression index is less than 0.9. This may be because the flow of O_2 depends on some variables that were assumed constant and or were not taken into account. To overcome this error and to reach more acceptable regression values it is necessary to perform more simulations and combinations of variables.

From the error distribution and doing a hypothesis test on the errors it can be stated that with a 95% certainty the absolute error of the data is between a 1 and 1.5% of error comparing the data from the software and the plant values, this is comparable to other studies[9] where absolute errors less than 5% were achieved using Aspen Hysys® software in natural gas plants.

As in other investigations[4], it was possible to simulate the cryogenic distillation stage, finding in our simulation a linear regression adjustment above 0.85. We also simulated a compression system finding a regression adjustment of 0.99. In other investigations we found absolute errors of between 1.5% and 1.3%[8]
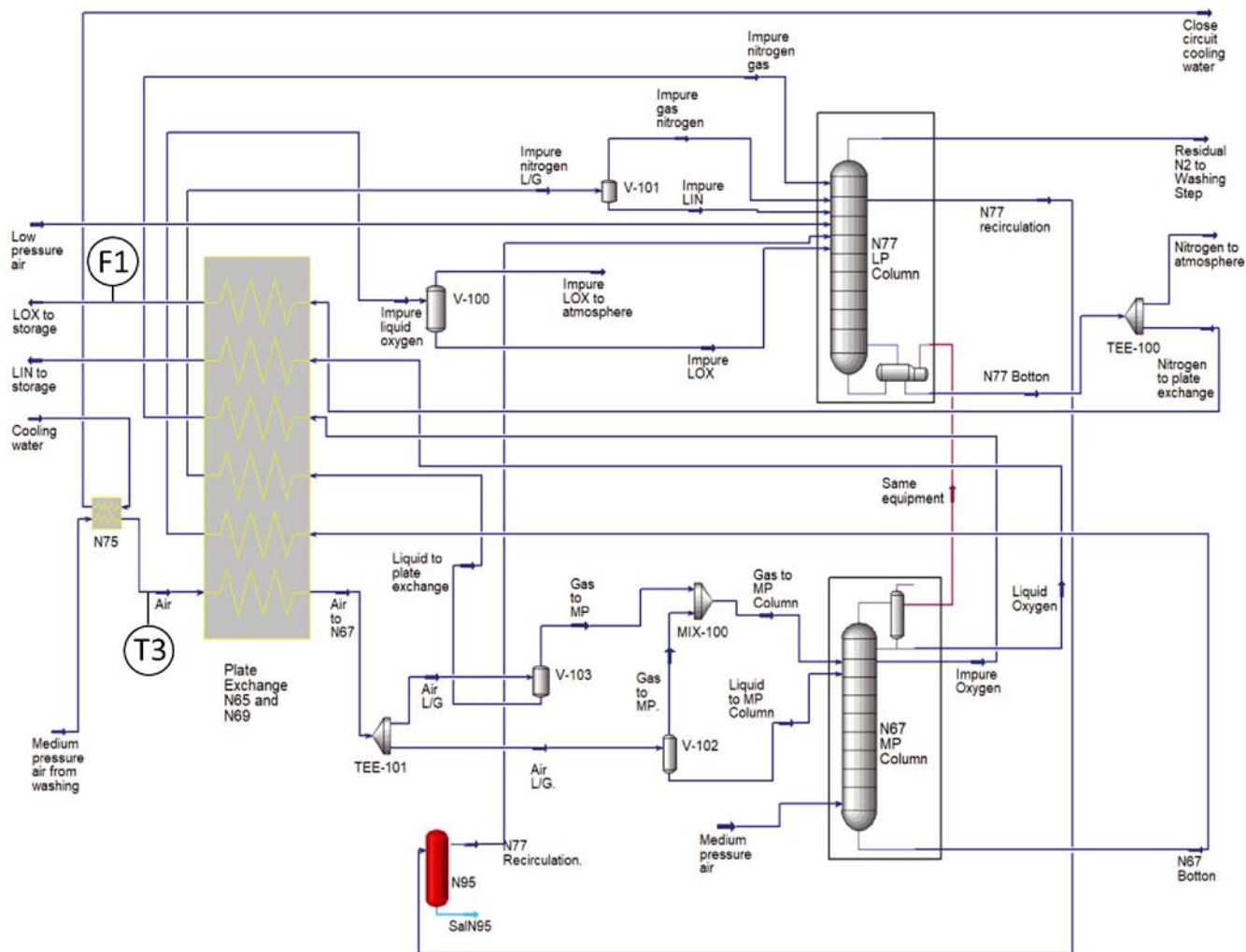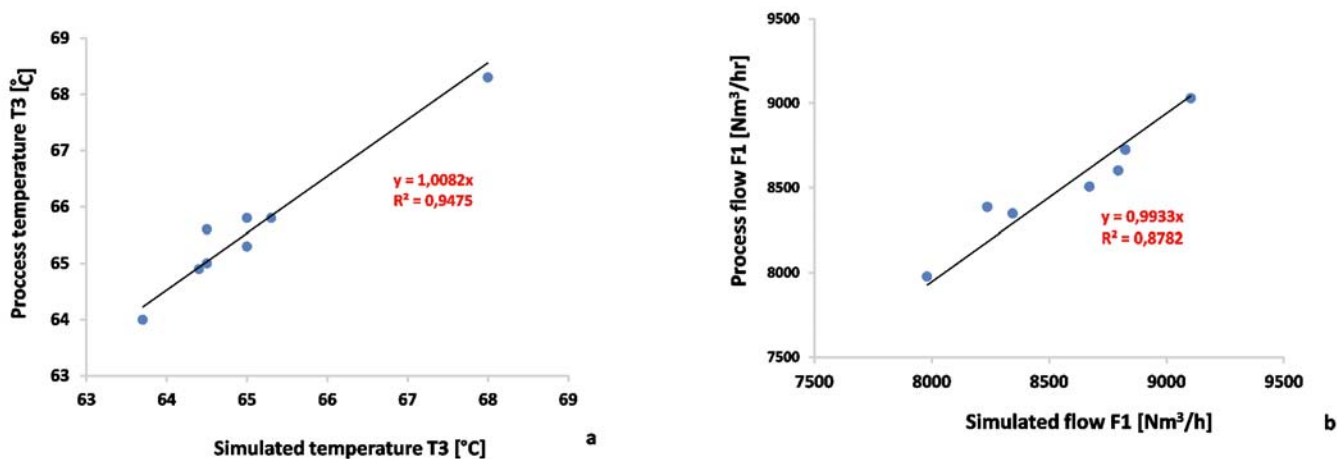
Figure 7. Cold Box simulation flow sheet

Figure 8. Cold box results compression (a), and Cold box O_2 flow results (b)

CONCLUSION

Using operational data, a simulator was made for the Oxinor plant with the Aspen Hysys® software tool.

Validating the simulator with historical data of the plant shows that the errors between the process variables and the values delivered by it have values that fluctuates between 1% and 1.5%.

The use of this software allowed consideration of the main stages of the process, which allowed evaluation and

validation of parts each system, and the entire productive process, which consist of the following stages:
  – Compression;
  – Washed;
  – Second compression;
  – Cold box;
  – Compressor/turbine system; and
  – Water cooling plant.

Finally, the simulated tool was validated with the data of the Oxinor I plant, which allows it to be used
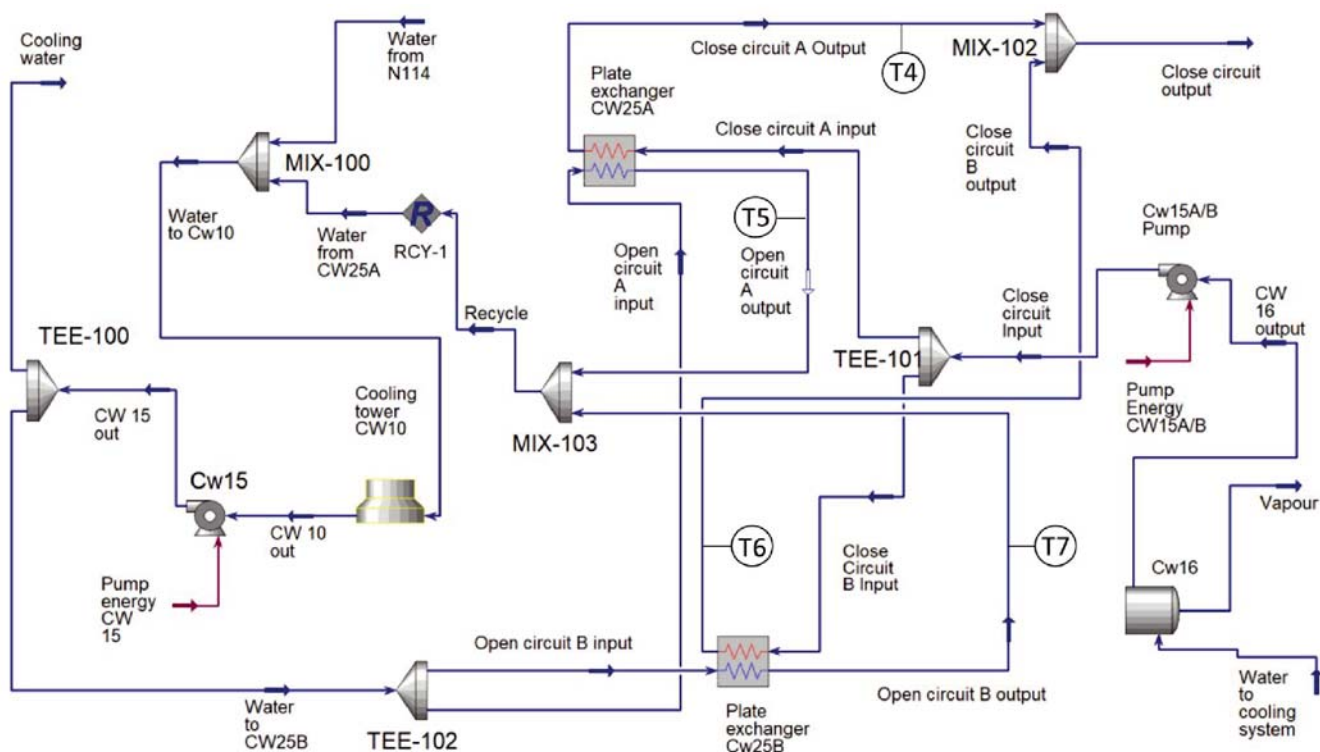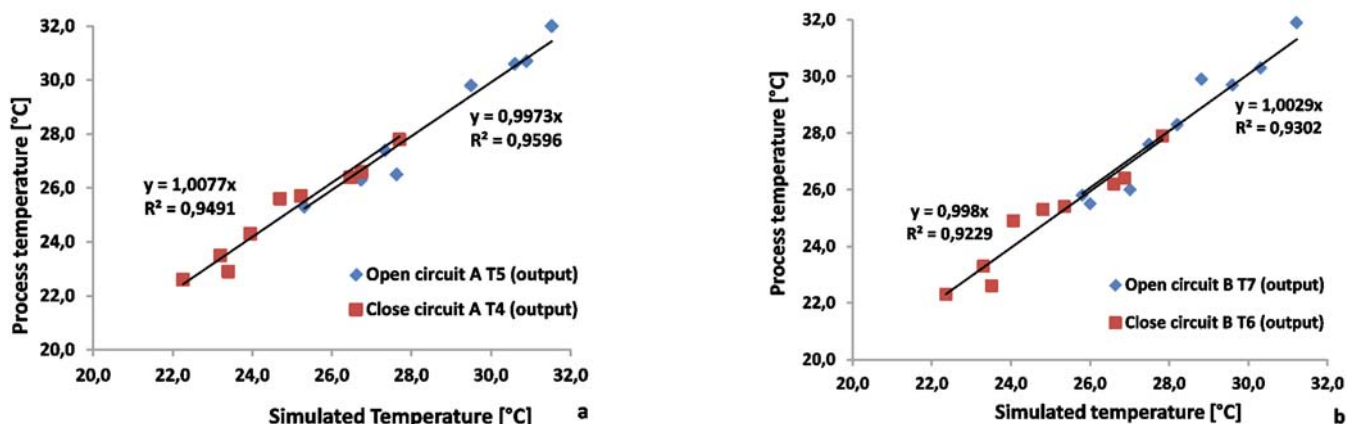
Figure 9. Water cooling plant simulation flow sheet

Figure 10. Water cooling plant results for outlet current circuit a and b
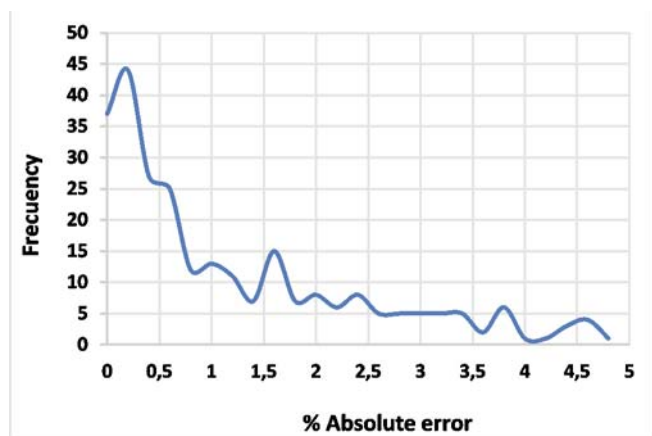

Figure 11. Error distribution chart

as a base tool to study any operational or equipment changes in this production process.

The simulated plant might also help with future works on the Air Liquide Chile S.A Oxinor I plant using the software Aspen Hysys® without wasting time and efforts on validating the software on the plant.

The authors of this paper consider the following topic for future research is: Process optimization of the oxynor cryogenics plant using the simulation developed in this work.

APPENDIX

Design Data information

Table 1. Compression design data

Air Compressor (3 step)	Design
Fluid	Air
Flow	47768 [Nm3/h]
Inlet Pressure	95.15 [kPa Absolute]
Inlet Temperature	20 [°C]
Relative Humidity	80 [%]
Discharge Pressure	484.0 [kPag]
Discharge Temperature	92.8 [°C]

Table 2. Tower N114 design data

Water Wash Tower N114	Design
Fluid	Air
Flow	47060 [Nm3/h]
Inlet Pressure	477.4 [kPag]
Inlet Temperature	92.8 [°C]
Inlet Relative Humidity	100 [%]
Outlet Pressure	474,4 [kPag]
Outlet Temperature	11.6 [°C]

Table 3. LOX production design data

LOX Production	Design
Fluid	Liquid Oxygen
Flow	9540 [Nm3/h]

Table 4. Cooling water interchange design data

Cooling water Interchange CW 25 A/B	Close Circuit Design	Open Circuit Design
Fluid	Water	Water
Flow	231.7 [Nm3/h]	231.7 [Nm3/h]
Inlet Pressure	318.5 [kPag]	249.6 [kPag]
Inlet Temperature	21.1 [°C]	31.9 [°C]
Outlet Temperature	29.4 [°C]	23.6 [°C]

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