STUDY OF CRYOGENIC CYCLES WITH ASPEN - HYSYS SIMULATIONS

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By

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CERTIFICATE

This is to certify that the project work entitled "Study of Cryogenic Cycles with ASPEN-HYSYS Simulations" by Sunil Manohar Dash has been carried out under my supervision in partial fulfillment of the requirements for the degree of Bachelor of Technology during session 2008-09 in the Department of Mechanical Engineering, National Institute of Technology, Rourkela and this work has not been submitted elsewhere for a degree.

Place: Rourkela Date: Prof. Sunil Kumar Sarangi Dept. of Mechanical Engg. Director, N.I.T. Rourkela. Rourkela.

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ABSTRACT

Computer-aided process design programs, often referred to as process simulators, flow sheet simulators, or flow sheeting packages, are widely used in process design. Aspen HYSYS by Aspen Technology is one of the major process simulators that are widely used in chemical and thermodynamic process industries today. It specializes on steadystate analysis. System simulation is the calculation of operating variables such as pressure, temperature and flow rates of energy and fluids in a thermal system operating in a steady state. The equations for performance characteristics of the components and thermodynamic properties along with energy and mass balance form a set of simultaneous equations relating the operating variables. The mathematical description of system simulation is that of solving these set of simultaneous equations which may be non-linear in nature.

Cryogenics is the branch of engineering that is applied to very low temperature refrigeration applications such as in liquefaction of gases and in the study of physical phenomenon at temperature of absolute zero. The various cryogenic cycles as LINDE cycle, CLAUDE cycle etc govern the liquefaction of various industrial gases as Nitrogen, Helium etc. The following work aims to simulate the cryogenic cycles with the help of the simulation tool ASPEN HYSYS where all calculations are done at steady state and the results hence obtained.

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CHAPTER-1

INTRODUCTION

Now a day the process industries are faced with an increasingly competitive environment, ever changing market conditions and government regulations. Yet they a still have to increase productivity and profitability. The business objective can be achieved by reducing time required to get new products to market, increasing the quantity and quality of product produced and designing plants for an optimum performance along their life cycle. In industries these complicated problems are often not solved by hand for two reasons.

- ➢ Human Error.
- Time constraints

There are many different simulation programs used in industry depending on the field of application and desired simulation product. When used to its full capability 'ASPEN' can be a very powerful tool for an engineer to achieve major business benefits.

- Ensuring more efficient and profitability design.
- Improving plant control, operability.
- Eliminating process bottle necks and minimizing process network.
- > Reducing human error and time requirement.

The inherent flexibility contributes through its design, combined with the unparallel accuracy and robustness provided by it, leads to represent a more realistic model. It can be used for variety of field including oil and gas production, refining, chemical processing, environment study, power generation, cryogenic applications.

1.1 Gas liquefaction systems

This chapter discusses several systems used to liquefy the cryogenic fluids. The performance of the various systems is specified by the system performance parameters or payoff functions.

1.2 System performance parameters

There are three payoff functions used to indicate the performance of the liquefaction systems:

- 1. Work required per unit mass of gas compressed.
- 2. Work required per unit mass of gas liquefied.
- 3. Fraction of the total flow of gas that is liquefied.

1.3 The thermodynamically ideal system

In order to have a means of comparison of liquefaction systems through the figure of merit, let first analyze the thermodynamically ideal liquefaction system. This system is ideal in the thermodynamic sense, but it is not ideal as far as practical system is concerned. The perfect cycle in thermodynamics is the Carnot cycle. Liquefaction is essentially an open system process consists of, a reversible isothermal compression followed by a reversible isentropic expansion. The gas to be liquefied is compressed reversibly and isothermally from ambient conditions to some high pressure. This high pressure is selected so that gas will become saturated liquid upon reversible isentropic expansion through the expander. The pressure attained at the end of isothermal compression is extremely high in the order of 70 Bars, which is the reason it is not an ideal process for a practicable system.

1.4 Production of low temperatures

1.4.1 Joule Thompson effect

Most of the practical liquefaction systems utilize an expansion valve or a Joule Thomson valve to produce low temperatures. If the first law of steady flow is applied to the expansion valve, for zero heat transfer and zero work transfer and for negligible kinetic and potential changes, gives h1= h2. There is a region in which an expansion through the valve produces an increase in temperature, while in another region the expansion results in a decrease in temperature. The expansion valve should be operated in liquefaction system in the region where there is a net decrease in temperature results. The curve that separates two regions is called the *inversion curve*. The effect of change in temperature for an isenthalpic change in pressure is represented by the *Joule-Thompson coefficient*.

1.4.2 Adiabatic expansion

The second method of producing low temperatures is the adiabatic expansion of the gas through a work producing device, such as an expansion engine. In the ideal case, the expansion would be reversible and adiabatic and therefore isentropic. In this case an isentropic coefficient is defined which expresses the temperature change due to a pressure change at constant entropy.

1.5 Existing Gas liquefaction systems

Of the various gas liquefaction techniques developed by various cryogenic experts, some of them are listed below:-

- 1: Linde System.
- 2: Claude System.
- 3: Kaptiza System.
- 4: Heylandt System.
- 5: Cascade System.

The following project work emphasizes on the two basic and widely used liquefaction systems i.e the Linde cycle and the Claude cycle for liquefaction of industrial gases.

CHAPTER-2

LITERATURE SURVEY

2.1 Thermodynamic and Cryogenic Cycles Review.

2.1.1 Thermo dynamic Cycles

A thermodynamic cycle is a series of thermodynamic processes which returns a system to its initial state. Properties depend only on the thermodynamic and thus do not change over a cycle. Variables such as heat and work are not zero over a cycle, but rather are process dependent. A thermodynamic process may be defined as the energetic evolution of a thermodynamic system proceeding from an initial state to a final state. Paths through the space of thermodynamic variables are often specified by holding certain thermodynamic variables constant.

Some of the thermodynamic processes are given below:

- An isobaric process is a thermodynamic process in which the pressure stays constant: $\Delta p = 0$.
- An isochoric process, also called an isovolumetric process, is a process during which volume remains constant.
- An isothermal process is a change in which the temperature of the system stays constant: $\Delta T = 0$.
- > A polytropic process is a thermodynamic process that obeys the relation:

 $PV^n = C$,

Where P is pressure, V is volume, n is any real number (the polytropic index), and C is a constant.

Some of the thermodynamics are: Carnot cycle, Ericsson cycle, Stirling cycle, Otto cycle.

2.1.2 Cryogenic Cycles

The field of cryogenics advanced during World War II when scientists found that metals frozen to low temperatures showed more resistance to wear. Cryogenic is the branch of physics and engineering that involves the study of very low temperature, how to produce them, how material behave to those temperature. A process is said to be cryogenic if the operating temperature is below -150° c or 123k. For most of cryogenic work the temp range lies between 4k -77k. Specifically Linde and Claude cycle is discussed for the present study.

<u>LINDE Cycle</u>

Linde cycle is a typical cryogenic cycle used for liquefaction of gases and is the simplest of all liquefaction cycle. The schematic of the cycle is shown below.



Figure 2.1 Showing line diagram of LINDE cycle.



Figure 2.2 Showing T~S diagram of LINDE cycle.

Components Used

- 1. *COMPRESSOR*: It is a device used to reduce the volume of gaseous air and increase the pressure. Generally for cryogenic application compressor with high compression ratio are used. To achieve high stage compression ratio a number of compressor are used in series rather using a single compressor. It also reduces work consumption. For present work isothermal compression process is used.
- 2. *HEAT EXCHANGER*: Heat exchangers are devices which transfer heat from hot fluid stream to cold fluid stream. In heat exchanger hot fluid temperature decreases and there is increase in temperature of cold fluid. By losing heat hot fluid is prepared for throttling process and similarly by gaining heat cold fluid heated up for compression process.
- **3.** *VALVE*: A throttling valve is used to reduce the pressure of the compressed air so that liquid air can be produced and stored. The process is assumed to be isenthalpic expansion.

- **4.** *SEPARATOR/DISTILLATION COLUMN*: In this chamber air is separated into desired components like liquid N₂, liquid O₂ etc and the gaseous part is again recirculated.
- **5.** *MIXER*: It is a device helps to maintain a constant flow rate of air into the compressor. The extra amount of air is added into incoming stream from separator. The process is assumed to be isobaric.

A basic differentiation between the various refrigeration cycles lies in the expansion device. This may be either an expansion engine like expansion turbine or reciprocating expansion engine or a throttling valve. The expansion engine approaches an isentropic process and the valve an isenthalpic process. Isentropic expansion implies an adiabatic reversible process while isenthalpic expansions are irreversible. In the Linde's system, the basic principle of isenthalpic expansion is also incorporated where as in Claude's cycle involves both isentropic and isenthalpic expansion procedure.

<u>CLAUDE Cycle</u>

The expansion through an expansion valve is an irreversible process thermodynamically speaking. Thus if we wish to approach closer to the ideal performance, we must seek a better process to produce lower temperatures. In the Claude system energy is removed from the gas stream by allowing it to do some work in an expansion engine or an expander. If the expansion engine is reversible and adiabatic, the expansion process is isentropic and a much lower temperature is attained than that for an isenthalpic expansion.



Fig 2.3 Showing a schematic of Claude Cycle with T~S diagram.

The Claude nitrogen liquefaction system differs from the simple Linde's system by the addition of an expander and a second heat exchanger. In this system, the nitrogen is compressed isothermally to approximately 40 atmospheric pressure between points 1 and 2 as in figure 2.3. The high pressure nitrogen is partially cooled by passing through the first heat exchanger between points 2 and 3.

A portion of nitrogen about 80 percent at point 3 is bled and cooled by expansion in an expander between points 3 and 8. The remaining portion passes through the second heat exchanger between points 3 and 4. The nitrogen from the second heat exchanger is throttled irreversibly between points 4 and 5 at atmospheric pressure. The liquid nitrogen is removed by the separator at point 6. The lower temperature nitrogen from the expander at point 8 is mixed with the unliquefied nitrogen from the separator at point 7, giving the increased mass flow of nitrogen at point 4. This nitrogen passes through the two heat exchangers to the compressors.

2.2 Applications of Cryogenics

- Cryogenic Technology is used for production of Gases for industrial and commercial applications. In this process liquefaction and purification of Helium, Nitrogen gases are done. Also using this technique production of inert gases is done.
- 2. Cryogenics is very crucial for aerospace application. This technology is very critical for wind tunnel testing application. High performance wind tunnel required rapid movement of Nitrogen gas around the aerodynamic circuit.
- Cryogenic is required for Frozen Food Industries for preservation of food item depending upon type of food item and whether they are cooked or not before freezing..
- 4. Cryogenic has got lot of application in medical field. It is wildly used in MRI equipment for diagnosis of diseases.
- 5. Cryogenic has got a great role in chilled water storage system.

In particular air separation process is discussed.

2.2.1 Air Separation Process

Cryogenic air separation process is one of the most popular air separation process used to produce purified components of air, in particular oxygen, nitrogen, and argon. In cryogenic gas processing various equipments like distillation column, heat exchanger, cold inter connecting pipes are used at very low temperature. Hence all these equipments must be well insulated. Process cycles are somewhat different depending upon how many products are desired (either nitrogen or oxygen; oxygen and nitrogen; or nitrogen, oxygen and argon); the required product purities; gaseous product delivery pressures; and whether one or more products will be produced and stored in liquid form.

Following are the steps for producing liquid gases.

- 1. Filtering and compressing the air. The compressed air is then cooled to close-toambient temperature by passing through water-cooled or air-cooled heat exchangers.
- 2. Removing the remaining water vapor and carbon dioxide. These components of air must be removed to meet product quality specifications. In addition, they must be removed prior the air entering the distillation portion of the plant. If they were not, very low temperatures would cause the water and carbon dioxide to freeze and deposit on the surfaces within the process equipment.
- 3. The next step is additional heat transfer against product and waste gas streams to bring the air feed to cryogenic temperature (approximately -300 degrees Fahrenheit or -185 degrees Celsius). This cooling is done in brazed aluminum heat exchangers which allow the exchange of heat between the incoming air feed and cold product and waste gas streams exiting the separation process.
- 4. Distillation columns are used to separate the air into desired products. To make oxygen as a product, the distillation system will have both "high" and "low" pressure columns. Nitrogen plants may have only one column, although many have two. Nitrogen leaves the top of each distillation column; oxygen leaves from the bottom. Argon has a boiling point similar to that of oxygen and will preferentially stay with the oxygen product. If high purity oxygen is required, argon must be removed from the distillation system at an intermediate point. Impure oxygen produced in the initial (higher pressure) column is further purified in the second, lower pressure column.
- 5. The cold gaseous products and waste streams that emerge from the air separation columns are routed back through the front end heat exchangers. As they are warmed to near-ambient temperature, they chill the incoming air.

Thus required liquid gases are produced for commercial application.



Figure 2.4 Process Flow diagram for air distillation process.

CHAPTER-3

NUMERICAL ANALYSIS

3.1 System Simulation

System simulation is the calculation of operating variables such as pressure, temperature, and flow rates, energy of fluids in a thermal system operating in a steady state. The equations for performance characteristics of the components and thermodynamic properties along with energy and mass balance form a set of simultaneous equations relating the operating variables. The mathematical description of system simulation is that of solving these simultaneous equations many of which are non-linear.

One of the most common techniques used in simulating complex systems is the sequential modular approach which is described subsequently.

3.2 Sequential Modular Approach

Sometimes it is possible to start with the input information and immediately calculate the output of a component. The output information from the first component is all that is needed to calculate the output information for the next component and so on to the final component of the system, whose output is the output information of the system. Such a system simulation consists of sequential calculations and hence the name sequential modular approach.

Other methods of simulations include the Successive substitution or the Gauss Seidel iterative technique and the Newton's Raphsons Technique.

The various system simulation techniques were thoroughly studied and applied to simulate some simple and complex systems which would be described subsequently.

For the present study Claude Cycle is discussed more specifically. The problem is to find out the yield of liquid nitrogen under given conditions.



Figure 3.1 Flow diagram for a simple Cryogenic Cycle working on the principle of Claude Cycle.

3.3 Solution Methodology

Let m_6 = yield of liquid N₂ in kg/s. m_2 = mass flow rate of N₂ compressed = 0.1Kg/s m_8 = mass flow rate of N₂ bypassed to the expander = 0.6m₂ = 0.06 kg/s. m_4 = mass flow rate of N₂ passing through the second heat exchanger $= m_2 - m_8 = 0.04$ kg/s.

Now that all the parameters defined and so also the variables, the set of simultaneous equations were set as follows.

1: ENTHALPY AT 8'

 $\eta_{\text{isentropic}} = 0.4$ (h₃-h_{8'}) = 0.4*(h₃-h₈)-----(1)

2: ENTHALPY AT 9

The air from expander at 8' is mixed with unliquefied air from the separator at point 7. The condition of air after mixing is represented by point 9 on T-S diagram. $h_9(m_2-m_6) = m_8*h_{8'} + (m_4-m_6)h_7$ ------(2)

3: HEAT BALANCE OF FIRST HEAT EXCHANGER

 $m_2(h_2-h_3)=(m_2-m_6)(h_1-h_{10})$ -----(3) Here we get h_9 as a function of m_6 .

4: HEAT BALANCE OF SECOND HEAT EXCHANGER

 $m_4(h_3-h_4)=(m_2-m_6)(h_{10}-h_9)-\dots(4)$

5: HEAT BALANCE OF THE SEPARATOR

 $m_4*h_5 = m_6*h_6 + (m_4-m_6)h_7$ -----(5)

6: ISENTHALPIC EXPANSION IN THE THROTTLING PROCESS

 $h_4 = h_5$ ------(6)

Based on the system of simultaneous equations various sequencing and iterative techniques were used to solve the unknowns i.e the temperatures and the enthalpies.

A number of simulation tools are available for numerically analyzing thermodynamic cycles. For the present work commercial software ASPEN HYSYS is used. It has got a strong foundation in thermodynamics. Also the package contains built in equations used in thermodynamic processes, transport properties of hydrocarbons, non hydrocarbons, and petrochemical etc.

CHAPTER-4

ASPEN-HYSYS AS THE PROCESS MODELLING TOOL

4.1 Aspen Hysys as the simulation tool

Aspen Hysys is a Process modeling tool for steady-state simulation, design, performance monitoring, optimization and business planning for chemicals, specialty chemicals, petrochemicals and metallurgy industries.

The Challenge: Understanding and Predicting Process Behavior

The chemical process industries are faced with an increasingly competitive environment, ever-changing market conditions, and government regulations; yet they still must increase productivity and profitability. Bottom line performance can be adversely affected by many factors, such as production economies and product quality. Many of these factors are extremely complex and subject to varying degrees of unpredictability. Process engineers routinely address these difficult issues. They are faced with challenges that range from the designing new processes to evaluating and improving performance of existing plants while they address these business objectives. Experience alone is not always sufficient to answer the questions that continually arise – and 'trial and error' efforts to provide meaningful insights are costly and potentially dangerous. To avoid production delays, downtime or off-spec product, process manufacturers require cost effective tools that help identify and 'correct' anticipated problems before they occur.

The Opportunity: Maximizing Plant Performance and Enhancing profitability

Fundamental to improving performance of the plant or enterprise, or even the extended supply chain, is an accurate representation of the basic processes. Companies need a product that will enable them to develop that information and then build the models required to optimize enterprise performance. Steady-state simulation is a powerful process engineering tool that enables engineers to simulate plant behavior and analyze their results rapidly – exploiting the latest software and engineering technology to optimize plant performance and profitability.

The Solution: Aspen Hysys

Aspen Hysys solves the critical engineering and operating problems that arise throughout the lifecycle of a chemical process, such as designing a new process, troubleshooting a process unit or optimizing operations of a full process like an Acrylic Acid plant. The process simulation capabilities of Aspen Hysys enables engineers to predict the behavior of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. With reliable thermodynamic data, realistic operating conditions and the rigorous Aspen Hysys equipment models, they can simulate actual plant behavior.

Benefits Offered by Aspen Hysys

Aspen Hysys has a proven track record of providing the chemical process industries with substantial economic benefits throughout the manufacturing lifecycle of a process, from R&D through engineering and into production. It brings the power of steady-state process simulation to the engineering desktop, and delivers both modeling power and ease of use. With Aspen Hysys, companies can design, simulate, troubleshoot and manage profitable process plants. For example:

- The R&D group has come up with a new process for manufacturing a commodity chemical. They have detailed physical and thermodynamic property data and have had successful pilot plant operations. How do you evaluate the commercial feasibility of using this process?
- The main process line has recently come up after a turnaround during which several de-bottlenecking operations were performed. However, the results are falling short of design. How do you explore the impact of key operating variables upon operation of the process line to see what can be done to improve performance?

Aspen Hysys Features

Aspen Hysys is a component of the Aspen Engineering Suite[™] (AES), an integrated set of products designed specifically to promote best engineering practices and to optimize and automate the entire innovation and engineering workflow process throughout your plant and across your enterprise. Automatically integrate process models with your engineering knowledge databases, investment analyses, production optimization and numerous other business processes. Aspen Hysys contains data, physical properties, unit operation models, built-in defaults, reports and other features and capabilities developed for specific industrial applications, such as electrolyte simulation. Key Aspen Hysys features are listed below:

- Windows® Interoperability. Interface contains a process flowsheet view for graphical layout, data browser view for entering data, the patented Next expert guidance system to guide the user through a complete and consistent definition of the process flowsheet.
- Plot Wizard. Enables the user to easily create plots of simulation results.
- Flowsheet Hierarchy and Templates. Collaborative engineering is supported through hierarchy blocks that allow sub-flowsheets of greater detail to be encapsulated in a single high-level block. These hierarchy blocks can be saved as flowsheet templates in libraries.

- Equation-Oriented Modeling. Advanced specification management for equation oriented model configuration and sensitivity analysis of the whole simulation or specific parts of it. The unique combination of Sequential Modular and Equation Oriented solution technology allows the user to simulate highly nested processes encountered typically in the chemical industry.
- Thermo physical Properties. Physical property models and data are key to generating accurate simulation results that can be used with confidence. Aspen Hysys uses the extensive and proven physical property models, data and estimation methods available in Aspen Properties[™], which covers a wide range of processes from simple ideal behavior to strongly non-ideal mixtures and electrolytes. The built-in database contains parameters for more than 8,500 components, covering organic, inorganic, aqueous, and salt species and more than 37,000 sets of binary interaction parameters for 4,000 binary mixtures.
- **Convergence Analysis** to automatically analyze and suggest optimal tear streams, flowsheet convergence method and solution sequence for even the largest flowsheets with multiple stream and information recycles.
- Sensitivity Analysis to conveniently generate tables and plots showing how process performance varies with changes to selected equipment specifications and operating conditions.
- **Design Specification** capabilities to automatically calculate operating conditions or equipment parameters to meet specified performance targets.
- **Data-Fit** to fit process model to actual plant data and ensure an accurate, validated representation of the actual plant.
- Determine Plant Operating Conditions that will maximize any objective function specified, including process yields, energy usage, stream purities and process economics.
- Simulation Basic Manager. This feature available in Aspen Hysys for using different fluids like nitrogen, air, acetylene as per requirement. Also several fluid packages like BWRS, MWRS, and ASME are provided to calculate properties at different states.

CHAPTER-5

ASPEN HYSYS SIMULATIONS

For the present study an attempt has made to simulate LINDE Cycle for liquefaction of Air and CLAUDE Cycle for liquefaction of Nitrogen. The details of two cycles are discussed below.

5.1 Problem Specifications

5.1.1 Problem no 1.

To represent LINDE cycle as shown in figure 2.1 using ASPEN HYSYS for the following given condition and calculate amount of liquid air is separated in the separator.

- 1) Mass flow rate of air 1 kg/hr at 1 bar pressure.
- 2) Compression Ratio 250:1.
- 3) Inlet temperature of air 27° C
- 4) After throttling valve pressure drops to 1.2 bars.
- 5) Iso Thermal compression process in compressor.
- 6) Iso Enthalpic throttling in Valve.

5.1.2 Process Flow Diagram

To represent above LINDE cycle in Aspen Hysys the first step is to make a process flow diagram (PFD). In Simulation Basic Manager a fluid package is to be selected along with the fluid which is to be cycled in the process. For the present work air is selected as fluid and BWRS as fluid package. Now using an option "Enter to simulation Environment" PFD screen is started. An object palette will appear at right hand side of the screen.

In the object palette a number of components available some are given below.

- i. Streams (Material/Energy streams)
- ii. Vessels (Separator and Tanks)
- iii. Heat Transfer Equipments (Heat exchanger, Valves)
- iv. Rotating Equipments.
- v. Piping Equipments.
- vi. Solid Handling.
- vii. Reactor.
- viii. Logical.
- ix. Sub Flow sheet.
- x. Short Cut Column.



Some of the components used.

T	6 7
P-100 2	gh
ecc	K-101
4 5 eccc K-100	

WhereP-100 is a centrifugal pump.K-100 is a compressor.K-101 is an expander.



Where

MIX-100 is a mixer. VLV-100 is a valve. LNG-100 is a LNG heat exchanger. V-100 3-phase separator. For every component certain inputs are supplied as constraints for the component operation. Some of the specifications are

- 1. For streams mass flow rate, temperature, and pressure.
- 2. For Compressor compression ratio, inlet and outlet streams, duty factor, adiabatic efficiency.
- 3. For Expander adiabatic efficiency, inlet and outlet streams, and work outputs.

After constraining every component properly the specific window gives a green signal and then Simulation is started. Following figure shows a partially solved process.



Figure 5.1 Shows partially solved LINDE cycle.

Above process is partially solved because all the streams are not in blue color (4, 5 streams). Following figure shows a solved LINDE cycle with all streams in blue.



Figure 5.2 Flowsheet for LINDE cycle created in Aspen Hysys.

5.1.3 Basic description of the flowsheet

The above flowsheet in Aspen Hysys shows the various components and the material streams needed to bring about the liquefaction of the air. It consists of a mixer, an isentropic compressor, a cooler, a shell and tube countercurrent heat exchanger, an isenthalpic J-T valve, a separator which performs flash operations and a splitter which takes care of the mass convergence problems. These components or the equipments are termed as the blocks in the language of Aspen Hysys.

5.1.4 The Process

A Fresh feed stream of air at 300K and 1.0 bar enters the mixer, goes through the compressor where both pressure and temperature both increases. The temperature of the output feed stream is usually in the order of >400 K and hence it has to be cooled before entering the shell and tube heat exchanger. Hence an intermediate after cooler is used so as to bring down the temperature of the hot fluid in the order of around 300 K. The hot fluid enters the tube side inlet whereby it is cooled down by the downstream shell side cold stream. Then it goes through an isenthalpic J-T valve whereby an isenthalpic flash results in decreasing the temperature of the fluid. The vapor fraction is usually of the order of 0.92 and it can be decreased or alternatively the cold can be increased taking care of the heat exchanger performance. The vapor liquid mixture which comes out of the valve enters the separator where the separator flashes the vapor liquid mixture and the desired liquid air can be collected from bottom. The remaining vapor rises and is directed towards the shell side of the heat exchanger where by its temperature increases. The out stream from the heat exchanger cannot be directly mixed with the feed stream as it results in some convergence problems. This can be taken care off by using a mixer with a specified mix fraction. This mixer purges a fraction of the recycled outlet stream from the heat exchanger and gradually mixes the whole of the incoming recycle stream with the fresh feed and the cycle goes on.

5.1.5 The components or the blocks or the equipments

The description of the various components and the conditions at which they operate are described subsequently.

a: Mixer (MIX-100)

The outlet and the inlet pressure to be the same = 1.0 bar inside the mixture whose main purpose is to mix two incoming streams and send the outlet stream at some intermediate and equilibrium state. We consider a fresh feed stream of Air entering the mixer at 300 K and 1.0 Bar at the rate of 1 Kg/hr and also the final recycle stream entering into it at the same pressure. These two streams mix and the output stream 1 goes to the compressor. The temperature estimate is roughly given a guess of 300 K.

b: Compressor (K-100)

The compressor is modeled to be isentropic with an isentropic efficiency of 85%. The discharge pressure is 250 bars and hence a pressure ratio of 250/1.0 is considered.

c: After Cooler(E-100)

The pressurized stream that comes out of the compressor is too hot to enter into the tube side of the heat exchanger and hence an after cooler with a flash specification of 300 K temperature and 250 bars is considered. There are no pressure drops inside it.

d: Heat exchanger(LNG-100)

The heat exchanger as used in the simulation is a countercurrent shell and tube heat exchanger where the hot fluid flows through the tube side and the cold fluid through the shell side. A pressure drop of 1 bar is occurring during the flow in hot stream and 0.2 bar in cold stream. The exchanger duty is given an initial guess a minimum temperature approach of 10 K is estimated.

e: J-T Valve(VLV-100)

An isentropic J-T valve is used in LINDE cycle which works at a constant enthalpy and is such that with decrease in pressure an appreciable drop in temperature is brought about. The specification given is with a calculation type of Adiabatic flash for specified outlet pressure and a pressure drop of 247.8 bars. The valid phases are vapor liquid mixture.

f: Phase separator(V-100)

For the purpose of flashing the vapor liquid mixture that comes out of the J-T valve, a phase separator is used with the flash specifications given with pressure =1.2 bar and a temperature of 90K which is just a guess value to start the iterative technique.

g: Recycler(RCY-1)

It is used for checking the convergence criteria. Generally at the place of under-constraint situation this is used to restrict the degree of freedom. After the convergence input and output conditions are with in the tolerance limit.

The inputs for the various blocks were given systematically including the guess values so that all the minimum informations were available and the simulation was ready to run.

The following data are available with us,

- 1: Temperature of feed=300 K
- 2: LP=1.0 bar in the LINDE cycle
- 3: HP=250 bar in the LINDE cycle
- 4: Mass flow rate of the feed stream=1 Kg/hr
- 5: Isentropic efficiency of the compressor=85%

Simulation results for the above LINDE cycle will be discussed in chapter-6. To increases the amount of liquefaction rate and efficiency of process some modification are made and an extra turbo expander is used along with a more Heat Exchanger. Detail specifications for CLAUDE cycle is mentioned as Problem no 2.

5.2.1 Problem no 2.

To represent CLAUDE cycle as shown in figure 2.3 using ASPEN HYSYS for the following given condition and calculate amount of liquid N_2 is separated and the optimum condition for maximum liquid output.

- 1. Operating Pressure (inlet) = 1 bar.
- 2. Compression Ratio 40:1.
- 3. Isothermal compression in compressor.
- 4. Inlet temperature N_2 of 27^0 C.
- 5. After throttling valve pressure drops to 1.3 bars.
- 6. Iso Enthalpic throttling in Valve.
- 7. Expander Efficiency varies from 0.4 to 0.6.
- 8. Fraction of liquid separated from main stream varies 0.6 to 0.8.
- 9. Volume flow rate of liquid N_2 is 300 nm³/hr.

Where 300 nm³/hr. can be converted to mass flow rate. It is found to be 0.11 Kg/s at a temp 300K. (From simple Gaseous principles).

5.2.2 Process Flow Diagram

To represent above CLAUDE cycle in Aspen Hysys the first step is to make a process flow diagram (PFD). In Simulation Basic Manager a fluid package is to be selected along with the fluid which is to be cycled in the process. For the present work N₂ is selected as fluid and BWRS as fluid package. Now using an option "Enter to simulation Environment" PFD screen is started. An object palette will appear at right hand side of the screen. Components like compressor, LNG heat exchangers, J-T Valve, 3-Phase Separator, Turbo expander, Mixer, Recyclers are selected to draw PFD. These components or the equipments are termed as the blocks in the language of Aspen Hysys. Following figure 5.3 shows flowsheet diagram of CLAUDE cycle.



Figure 5.3 Showing the Claude cycle using ASPEN Hysis.

5.2.3 The Process

A Fresh stream of N_2 at 300K and 1.0 bar is feed into the mixer, which passes through the compressor where both pressure and temperature both increases. The temperature of the output feed stream is usually in the order of >400 K and hence it has to be cooled before entering the LNG heat exchanger. Hence an intermediate after cooler is used so as to bring down the temperature of the hot fluid in the order of around 300 K. The hot fluid enters the tube side inlet whereby it is cooled down by the downstream shell side cold stream. Now it passes through a splitter (TEE) where fraction of fluid is separated from main stream and passes through expander. This fraction varies from 0.6 to 0.8 of main stream fluid. Also for case studies expander adiabatic efficiency varies 0.4 to 0.6. The remaining portion of fluid goes through other two heat exchangers. Then through an isenthalpic J-T valve whereby an isenthalpic flash results in decreasing the temperature of the fluid. The vapor liquid mixture which comes out of the valve enters the separator

where the separator flashes the vapor liquid mixture and the desired liquid N_2 can be collected from bottom. The remaining vapor rises and is directed towards the shell side of the heat exchanger where by its temperature increases. The out stream from the heat exchanger (HX-3) get mixed with the expanded stream coming from expander and passes through the other two heat exchangers. The out stream from the heat exchanger cannot be directly mixed with the feed stream as it results in some convergence problems. This can be taken care off by using a mixer with a specified mix fraction. This mixer purges a fraction of the recycled outlet stream from the heat exchanger and gradually mixes the whole of the incoming recycle stream with the fresh feed and the cycle goes on.

5.2.4 The components or the blocks or the equipments

The description of the various components and the conditions at which they operate are described subsequently.

a: Mixer (MIX-1, MIX-2)

The outlet and the inlet pressure to be the same = 1.0 bar inside the mixture (MIX-1) whose main purpose is to mix two incoming streams and send the outlet stream at some intermediate and equilibrium state. A fresh feed stream of N_2 entering the mixer at 300 K and 1.0 Bar at the rate of 0.1 Kg/s and also the final recycle stream entering into it at the same pressure. These two streams mix and the output stream 1 goes to the compressor. The temperature estimate is roughly given a guess of 300 K. In the other mixture (MIX-2) the streams coming from expander and third heat exchanger mixes.

b: Compressor

The compressor is modeled to be isentropic with an isentropic efficiency of 85%. The discharge pressure is 40 bars and hence a pressure ratio of 40/1.0 is considered.

c: After Cooler(E-100)

The pressurized stream that comes out of the compressor is too hot to enter into the tube side of the heat exchanger and hence an after cooler with a flash specification of 300 K temperature and 40 bars is considered. There are no pressure drops inside it.

d: Heat exchanger(HX-1, HX-2, HX-3)

The heat exchanger as used in the simulation is a countercurrent shell and tube heat exchanger where the hot fluid flows through the tube side and the cold fluid through the shell side. A pressure drop of 0.1 bars occurring during the flow in each stream. The exchanger duty is given an initial guess a minimum temperature approach of 10 K is estimated.

e: Splitter(TEE-100)

Stream 3 coming from HX-1 is passed through splitter which separates a definite fraction of (0.6 to 0.8) fluid from main stream and allowed to bled later stage. The remaining portion of the fluid moves through other heat exchangers. This separation helps to achieve lower temperature and desired output conditions.

f: J-T Valve

An isentropic J-T valve is used in CLAUDE cycle which works at a constant enthalpy and is such that with decrease in pressure an appreciable drop in temperature is brought about. The specification given is with a calculation type of Adiabatic flash for specified outlet pressure and a pressure drop of 38.4 bars. The valid phases are vapor liquid mixture.

g: Phase separator

For the purpose of flashing the vapor liquid mixture that comes out of the J-T valve, a phase separator is used with the flash specifications given with pressure =1.3 bar and a temperature of 90K which is just a guess value to start the iterative technique.

h: Expander

It a rotating device used for expansion of separated fluid in the splitter. The expansion process is assumed to be isentropic. Adiabatic efficiency of expander is varied from 0.4 to 0.6 for different case studies.

i: Recycler(RCY-1, RCY-2, RCY-3, RCY-4, RCY-5)

It is used for checking the convergence criteria. Generally at the place of under-constraint situation this is used to restrict the degree of freedom. After the convergence input and output conditions are with in the tolerance limit.

The inputs for the various blocks were given systematically including the guess values so that all the minimum information was available and the simulation was ready to run.

The following data are available with us,

- 1: Temperature of feed=300 K
- 2: LP=1.0 bar in the CLAUDE cycle
- 3: HP=250 bar in the CLAUDE cycle
- 4: Mass flow rate of the feed stream=0.1 Kg/s
- 5: Isentropic efficiency of the compressor=85%
- 6: Expander efficiency = 0.4, 0.5, 0.6.
- 7: Fraction of fluid separated = 0.6, 0.62, 0.64, 0.66...etc.

Simulation results for the above CLAUDE cycle will be discussed in chapter-6. Also a comparison between LINDE and CLAUDE cycle is done to show the more efficient process of liquefaction.

CHAPTER-6

RESULTS AND DISCUSSIONS

In this chapter simulation results for both LINDE and CLAUDE are discussed separately and later a comparison is made between those to verify which cycle is better for liquefaction process.

6.1 LINDE Cycle Simulation Results.



Figure 6.1 showing the PFD of LINDE Cycle

As previously discussed the objective is to find out amount of liquid air output (stream 6). The details of mass flow rate, temperature, vapor fraction, pressure are given in tabulated format below.

Material Streams						
		1	2	3	4	5
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	0.9444
Temperature	к	290.50	1592.8	300.00	170.87	79.159
Pressure	bar	1.000	250.0	250.0	249.0	1.200
Molar Flow	kgmole/h	3.570e-002	3.570e-002	3.570e-002	3.570e-002	3.570e-002
Mass Flow	kg/h	1.0000	1.0000	1.0000	1.0000	1.0000
Liquid Volume Flow	m3/h	1.240e-003	1.240e-003	1.240e-003	1.240e-003	1.240e-003
Heat Flow	kW	-2.275e-003	0.4207	-8.711e-003	-6.620e-002	-6.620e-002
		6	7	8	9	10
Vapour Fraction		0.0000	1.0000	1.0000	1.0000	1.0000
Temperature	к	79.159	79.159	79.161	290.00	300.00
Pressure	bar	1.200	1.200	1.200	1.000	1.000
Molar Flow	kgmole/h	1.984e-003	3.371e-002	3.391e-002	3.391e-002	1.785e-003
Mass Flow	kg/h	5.5585e-002	0.94441	0.95000	0.95000	5.0000e-002
Liquid Volume Flow	m3/h	6.893e-005	1.171e-003	1.178e-003	1.178e-003	6.201e-005
Heat Flow	kW	-6.764e-003	-5.944e-002	-5.979e-002	-2.299e-003	2.363e-005

TABLE 1 Showing Results obtained from Aspen Hysys.

From above table amount of liquid air produced is given by column 6.

Mass flow rate of Liquid air:5.558e-2 Kg/hr.Pressure:1.2 Bar.Temperature:79.159 K.Vapor Fraction:0.0Mass flow rate of Liquid air
Total Mass flow rate=(0.05/1.0);= 5 % Liquefaction.

6.1.1 GRAPHS:-



(Temperature Vs Heat flow)

Figure 6.2 Plot showing Temp vs Heat flow rate for Heat Exchanger.



(Temperature Vs Delta T)

Figure 6.3 Plot showing Temp vs Delta Temp for Heat Exchanger.

(Temperature Vs UA)



Figure 6.4 Plot showing Temp vs Overall Conductance for Heat Exchanger.

Graphs are plotted between Temperature Vs Delta T, Temperature Vs Heat flow; Temperature Vs UA for LNG heat exchanger and the nature of curves for hot and cold composites are well comparable. In every case minimum temperature between hot and cold stream is 10° C which is well satisfied with our initial guess.

6.2 CLAUDE Cycle Simulation Results.



Figure 6.5 showing the PFD of CLAUDE Cycle.

CLAUDE Cycle is the modified cycle used for liquefaction with some extra components. The objective is to find out amount of liquid N_2 produced and the optimum amount of separation in the splitter for different adiabatic efficiency of expander.

Attach the pics.....newclaude2.pdf

Above table shows the optimum flow rate condition for expander efficiency 40% and separation through splitter is 0.68 of the main stream fluid. The column 7 shows the amount of liquid N_2 produced.

	= 27 % of liquefaction.
in main stream after separation)	
(Total Mass flow rate of liquid N ₂	
Mass flow rate of liquid N ₂	= (0.00864/0.032)
Pressure	: 1.3 bars.
Vapor fraction	: 0.0
Temperature	: 79.55 K
Mass flow rate of liquid N ₂	: 8.635e-003 kg/s.

Now the graphs are plotted to know the temperature variation of three Heat Exchangers used. Those are shown below.

6.2.1 GRAPHS

(For HX.1)



Figure 6.6 Plot showing Temp vs HeatFlow for Heat Exchanger -1.

(For HX-2)



Figure 6.7 Plot showing Temp vs HeatFlow for Heat Exchanger -2

(For HX.3)



Figure 6.8 Plot showing Temp vs HeatFlow for Heat Exchanger -3.

Above graphs show that in all heat exchanger minimum approach is 10K. Also the variation of temperature is well comparable with the theoretical results. It should be noted that in HX-3 the hot stream temp reduction is very less (<10K). This gives a idea for the future work for completing the CLAUDE cycle with out HX-3.

As mentioned earlier a number of simulations are done by varying the efficiency of turbo expander. Those are discussed as different Cases in following. The objective of present work is to find out optimum condition for maximum liquefaction.

Case1: (Expander adiabatic efficiency 40%)

Fraction of flow in main	Liquid N ₂ in Kg/s.
stream(3") after separation in	
splitter.	
0.28	8.21E-03
0.3	8.35E-03
0.32	8.64E-03
0.34	8.58E-03
0.36	8.27E-03
0.38	8.21E-03
0.4	7.96E-03
0.42	7.96E-03
0.44	7.82E-03
0.46	7.63E-03

From above table the mass flow rate is found maximum for the fraction of separation 0.32. An excel plot is made using above data to show the peak value.



Figure 6.9 Excel Plot of liquid N_2 o/p with fraction of N2 passing through stream 3".

Case2:	(Expander	adiabatic	efficiency	50%)
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Fraction of flow in main	Liquid N ₂ in Kg/s.
stream(3") after separation	
in splitter.	
0.32	9.40E-03
0.34	9.80E-03
0.36	1.05E-02
0.38	1.03E-02
0.4	1.03E-02
0.45	9.70E-03
0.5	9.18E-03



Figure 6.10 Excel Plot of liquid N_2 o/p with fraction of N2 passing through stream 3".

An excel plot is made using above data which show the maximum output is at 0.36 fraction of separation.

Case3: (Expander	adiabatic efficiency 6	60%)
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Fraction of flow in main	Liquid N ₂ in Kg/s.
stream(3") after separation	
in splitter.	
0.34	1.16E-02
0.36	1.20E-02
0.38	1.23E-02
0.4	1.19E-02
0.45	1.14E-02
0.5	1.09E-02
0.55	1.00E-02
0.6	9.37E-03



Figure 6.11 Excel Plot of liquid N₂ o/p with fraction of N2 passing through stream 3".

An excel plot is made using above data which show the peak value is at 0.38 fraction of separation. So the process should be operated at this condition for maximum productivity.

Now a single graph is made by combining all above three graphs which is shown below.



Figure 6.12 Excel Plot of liquid N₂ o/p with fraction of N2 passing through stream 3".

Also if a graph is made for different turbo expander efficiency and maximum liquefaction of N_2 the variation is found to be increasing with efficiency.

Turbo Expander Efficiency	Maximum Liquid output
	in Kg/s
0.4	8.64E-03
0.5	1.05E-02
0.6	1.23E-02



Figure 6.13 Excel Plot of liquid N₂ o/p with Turbo expander efficiency.

Therefore for better result higher adiabatic efficient turbo expander is used.

6.3 Comparison between LINDE and CLAUDE Cycle

In section 6.1 (LINDE Cycle) the ratio of liquid mass flow rate to total mass flow rate in main stream is found to be only 5%, where as in section 6.2 (CLAUDE cycle) this ratio is 27 %. This indicates that CLAUDE cycle is more efficient than LINDE cycle.

CHAPTER-7

CONCLUSION

7.1 Summery of the Work Done

Simulation of cryogenic cycles was done using the commercial software ASPEN HYSYS. In the present work Cryogenic cycles like LINDE cycle was used for liquefaction of air which yields only 5 % of liquid air at the end of the process. To increase the productivity one more modified cycle was used know as CLAUDE cycle where the liquefaction rate increases to 27 %. Also the work was extended to study CLAUDE with different adiabatic efficiency condition of the expander and optimum condition for the maximum liquid output was found out. Detailed graphical representations of various cases were also done.

7.2 Future Scope.

This project work simulates a LINDE cycle, CLAUDE Cycle using the simulation tool ASPEN HYSYS. The results obtained from simulation will helps to carry out experiments in lab at optimum condition and in later stages comparison can be made. Much complex cycles like the Kaptiza cycle, Heylandt Cycle, Collins liquefaction cycle for liquefaction of Nitrogen can also be simulated using the same ASPEN HYSYS. User defined functions can also be incorporated to solve complex real life simulations.

CHAPTER-8

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