DESIGN AND ECONOMIC FEASIBILITY OF NITROGEN PRODUCTION FROM AIR TECHNOLOGY [COMBUSTION-BASED]

By

Sadia Faizan

Ayesha Noor

Junaid Rana

Umair Butt

School of Chemical and Materials Engineering

National University of Sciences and Technology

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By

Leader – 343092 Sadia Faizan

Member-1 – 348035 Ayesha Noor

Member-2 – 336673 Junaid Rana

Member-3 – 334823 Umair Butt

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CERTIFICATE

This is to certify that work in this thesis has been completed by **Ms. Sadia Faizan, Ms. Ayesha Noor, Mr. Junaid Rana** and **Mr. Umair Butt** under the supervision of **Dr. Umair Sikandar** at the School of Chemical and Materials Engineering (SCME), National University of Science and Technology, H-12, Islamabad, Pakistan.

Advisor:

Dr. Umair Sikandar

Assistant Professor
School of Chemical and
Materials Engineering (SCME)
NUST, Islamabad (Pakistan)

Department of Chemical Engineering

School of Chemical and Materials

Engineering

National University of Sciences and

Technology

Submitted Through:

HOD: **Dr. Erum Pervaiz**

Dr. M. Bilal Khan Niazi
Professor, PhD
Chemical Engineering
SCME, NUST, Islamaba

Department of Chemical Engineering

School of Chemical and Materials

Engineering

National University of Sciences and

Technology

29-5-2024

Principal/Dean: **Dr. Amir Azam Khan**

Department of Chemical Engineering

School of Chemical and Materials

Engineering

National University of Sciences and

Technology

DEDICATION

This work is dedicated to our parents for always believing in us, our teachers, for broadening our *perspective of the world and our tireless hard work.*

ACKNOWLEDGEMENT

We want to start by expressing our sincere gratitude to the Almighty for His immense kindness. We understand that without His guidance and blessings, our project wouldn't have been a success. His mercy has truly been our guiding light throughout this endeavor.

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ABSTRACT

To design and find the economic feasibility of the novel combustion-based nitrogen production process. As the major challenge of any process to be feasible is its results and economy. Nitrogen production plant design and economic calculation of combustion- based method will be done. As the conventional methods for nitrogen production, PSA and Liquefaction, are highly energy intensive. This project overcomes the high energy requirements. As the name suggests, combustion-based technology, this generates energy, along with nitrogen. On the basis of exothermic reaction, which eventually is utilized by the process.

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CHAPTER 1

INTRODUCTION

1.1 Applications of nitrogen:

Nitrogen is an essential element for life, and it constitutes a significant portion of the Earth's atmosphere, has garnered immense importance in industrial processes due to its inert nature and widespread applications. Nitrogen gas (N_2) makes up about 78% of the atmosphere; it is often required in pure or concentrated forms for various industrial applications. The production of nitrogen involves separating it from the air, where it exists as a diatomic molecule (N_2).

There are several uses of Nitrogen (N_2), some which are as following:

- Chemical Industry, nitrogen is a crucial component for the synthesis of ammonia, which is the foundation for fertilizers, explosives, and various chemicals.
- Food Industry, nitrogen is used for packaging to prevent oxidation and spoilage, extending the shelf life of products. It is used as a preservative. Applications in freezing, chilling and inerting during food processing.
- Electronics and semiconductors, nitrogen is essential in the production of electronic components and semiconductors devices, providing an inert atmosphere to prevent oxidation during manufacturing processes.
- Metallurgy, nitrogen is used for purging and blanketing in metallurgical processes, preventing oxidation, and ensuring the quality of metal products by maintaining controlled atmospheres.
- Oil and gas Industry, nitrogen is employed for various purposes, including inerting storage tanks, enhancing oil recovery, and preventing combustion during drilling operations.

The reason Nitrogen is used most of time are as it is cost effective, as industrial scale nitrogen production methods are efficient and cost-effective, ensuring a reliable and affordable supply of nitrogen for various industrial applications. Nitrogen’ inert nature is also one of the reasons and it makes it a safe option for various industrial applications, reducing the risk of combustion and other hazards. Moreover, nitrogen production processes allows for precise control over the purity of nitrogen, meeting the specific requirements of different applications. Nitrogen has a minimal environmental impact, as its production methods are designed to minimize environmental impact with advancements focusing on energy efficiency and reduced greenhouse gas emissions.

CHAPTER 2

LITERATURE REVIEW

2.1 Pressure Swing Adsorption (PSA):

PSA is a widely used technique for producing nitrogen, usually giving the N_2 purity ranging from 95% to 99%, especially in industries and laboratories. It operates based on the principle of selective adsorption of gases onto solid surfaces. Zeolite or Carbon-molecular sieve materials are commonly used as absorbents. The process involves two alternating columns filled with absorbent material. Air is passed through one column at high pressure, allowing nitrogen to be absorbed while other gases (e.g. Oxygen) are expelled. When the adsorption column reaches saturation, the process switched to the other column. The saturated column is depressurized, releasing the adsorbed nitrogen. The process requires lesser energy consumption but the purity of nitrogen is affected at larger flow rates.

The nitrogen generation system using PSA boasts several strengths that make it a favorable choice for various applications. Firstly, it ensures high purity, with PSA yielding nitrogen at levels ranging from 95% to 99.9999%, making it particularly suitable for scenarios where minimal oxygen or moisture content is crucial. Additionally, the system is cost-effective, operating economically by utilizing air as feedstock without the need for extra chemicals. Its energy efficiency is noteworthy as it leverages pressure swings for efficient adsorption and desorption, effectively minimizing energy consumption. The compact and modular design of the PSA method allows for easy integration across diverse industries. Moreover, PSA method is recognized for its reliability, requiring low maintenance, possessing an extended lifespan, and ensuring a continuous nitrogen supply. However, like any technology, the PSA nitrogen generation system does have its limitations. Notably, it is not suitable for high-volume nitrogen production due to limited capacity. The system's performance is also influenced by the quality of the feed gas (air), necessitating pretreatment to address contaminants for an effective adsorption process. The purity of the nitrogen produced may vary due to fluctuations in certain parameters, introducing a degree of variability. The design and optimization of the PSA system can be complex, demanding precise control and continuous monitoring. Finally, a potential drawback is the high initial investment, which may pose a hurdle for smaller-scale applications, despite the long-term benefits offered by the system.

2.2 Cryogenic Distillation:

Cryogenic distillation is similar to fractional distillation but is more focused on producing high-purity nitrogen. Air is partially liquefied by compression, cooling and throttling. Separation is based on the boiling points. The process involves cooling air to extremely low temperatures, often below -196 ˚C, where all components of air become liquids. The liquid air is then fractionally distilled to separate nitrogen from other components. This method is particularly suitable for applications requiring ultra-pure nitrogen, such as in the semiconductor industry.

Cryogenic distillation stands out as a robust nitrogen generation method, boasting several strengths that cater to diverse industrial requirements. One of its primary advantages lies in achieving exceptional purity levels, often surpassing 99.99%. This attribute makes cryogenic distillation well-suited for various applications, including critical sectors such as food packaging, electronics, and healthcare. Furthermore, the technology demonstrates high efficiency, with recovery rates typically exceeding 90%, leading to substantial nitrogen gas production from the input air. Its reliability is underscored by a well-established and proven track record in various industrial settings. Additionally, the scalability of cryogenic distillation allows it to adapt to specific production needs, accommodating both small-scale applications like laboratories and larger industrial processes. Beyond its nitrogen capabilities, cryogenic distillation can recover and liquefy other air components like oxygen and argon, minimizing waste and contributing to environmental sustainability. However, cryogenic distillation does have certain limitations that need consideration. The process is energy-intensive, demanding substantial energy to achieve cryogenic conditions, which may impact economic viability in some cases. Its complexity, involving intricate equipment, can result in higher maintenance and operational costs. The technology also requires a large footprint, posing a challenge in limited land areas. Longer start-up times are another drawback, given the time required to reach the necessary operating temperature. Some nitrogen loss during startup and shutdown phases affects overall efficiency. Additionally, cryogenic distillation is ideally suited for high-purity nitrogen, and other methods should be considered for applications with lower purity requirements.

Many processes has been developed for nitrogen production that includes pressure swing adsorption, cryogenic distillation and combustion method. As for this project the combustion-based method is designed and simulated in detail. This project will present a comparative analysis of economic feasibility and percentage purity of nitrogen, of all three techniques.

2.3 Nitrogen Production by Combustion-based method:

A novel technology to produce nitrogen. The method is more commonly named as *"Chemical Looping Combustion (CLC*)" This technology was introduced in 1990-2000 and is still under research. The specialty of the process is it is integrated with a power plant, so along with nitrogen production power generation also takes place, which can be used anywhere in the ammonia plant. The major advantage of this process is that its cost effective, as PSA and cryogenic distillation are highly energy intensive processes. PSA requires a lot of compression power to compress air for the adsorption process in further. whereas cryogenic distillation requires a strong refrigeration cycle to liquefy gases in the air such as nitrogen, argon, oxygen etc. The capital cost as well as the operational cost of PSA and cryogenic distillation is more than combustion-based nitrogen production technique. To over-come the energy required by the other two processes, the combustion-based method has been introduced across the world, which introduces integration of nitrogen production from air, with a power plant. Green power can be produced, with high carbon capture rate and almost zero carbon emissions through this method.

CHAPTER 3

PROCESS SELECTION

3.1 Methodology:

The method employs two fluidized bed reactors, air (as source for nitrogen), fuel (as name suggests it is a combustion-based method), Oxygen carriers (usually powdered metal particles), as the compressed air enters first fluidized bed reactor the oxygen carrier particles (which are metal based) immediately oxidizes by reacting with the oxygen present in air, as the metal has the tendency to oxidized immediately as it comes in contact with the oxygen. This is an exothermic and irreversible process. The conversion according to experiments and literature review is found to be 99%. The contains now mainly N_2 with some trace impurities. The metal (i.e. M) oxidizes in the first reactor by reacting with the oxygen in air and becomes MO (metal-oxide). This metal oxide has to be reduced to metal again for nitrogen production in next cycle. The metal-oxide is reduced by reducing agent (that is fuel CH_4). The methane itself oxidizes (combusts) and reduces the metal-oxide to metal only particles which is again sent to first reactor for oxidation. In this way the metal particles oxidize itself, removes oxygen from the air, leaving behind nitrogen stream with some traces. This pure nitrogen is used in ammonia production. The traces usually contain argon (which is part of air. 1%), argon is inert and does not influence the Haber-Bosch process for ammonia production. As the process is combustion-based and due to exothermic reactions, high pressure and high temperature gases, power generation can also be done via turbines. N_2 gas stream and flue gas stream is passed through the turbine. Initially the streams are at 30 Bar, on downstream the pressure is about 5 bar, so these gaseous streams are capable of generating energy. As this process does not require energy, rather generates some KW energy per kg of N_2 produced. The reducing agent is methane. Other fuels can be used as well, but for least carbon generation, methane is the most useful. For energy optimization, waste heat recovery system can also be installed, (which is optional), a steam engine is employed extending the process, this uses the waste heat of downstream gases of turbine to generate further energy. The steam engine comprises of the equipment i.e. waste heat boiler, steam turbine, condenser, pump. The nitrogen gas is stored in a vessel, which is then further used for the ammonia production. As every industry has their respective power plants for energy generation equivalent to the requirements of operational energy for plant. This process has the benefit that the N_2 production plant is integrated with a power plant. This technology is still under study. It is at lab scale across different countries worldwide. It has been commercialized.

CHAPTER 4

PROCESS DESCRIPTION

4.1 Process:

4.1.1 Air Compressor:

The compressor is used to compress the air, the air is sourced from the open atmosphere, the compression of air is up till 30 bars, to run turbines in proceeding steps. This is a multi-stage compression. Three stage compression takes place, because the increase in pressure from 1 to 30 bar is high. Also, the flow rate of air is higher than natural gas, so the stages required are more. The multi-stage compressor is employed with interstage coolers to lower the temperature of the air after first compression and to decrease the compression load in second compression stage. As low temperature of gas makes the compression easier.

4.1.2 Fuel Compressor:

Fuel here is considered as natural gas, for ease in calculation it is considered pure methane, the traces are neglected. The compression here is from 1 to 30 bars. This is a multi-stage compression as well. (2 stage compression), employed with an interstage cooler. The cooling medium is the cooling water circulating, through heat exchangers.

4.1.3 Air Reactor (oxidizer):

The compressed air enters to the air reactor, this is also known as the oxidizer. This is a fluidized bed reactor, and powdered nickel is introduced in the reactor. This metal particles works as oxygen carrier and removes oxygen from the air. The metal nickel has the high tendency to oxidize, as it is exposed to air, it oxidizes, and Ni converts to NiO. The conversion is usually around 99% as the reaction is rapid and irreversible. The Ni particles are oxidized with the aid of air flowing. The reaction is highly exothermic and is favored at. The stream leaves the reactor and enters the cyclone separator, in order to separate NiO and N_2. The temperature cannot exceed from 1200C because beyond this temperature Ni particles melt, and this results in process failure. If the flow rate of air is such high that the heat released during reaction causes the temperature to exceed from 1200C, more than one fluidized bed reactors are employed.

4.1.4 Fuel Reactor (reducer):

The NiO formed in the air reactor is immediately reduced to NiO as it gets into the fuel reactor, the regeneration of Ni is important as it is responsible to remove the oxygen molecules from the air is next cycle. In this way the Ni keeps on circulating from air to fuel reactors. Ni is continuously oxidized and reduced in the respective reactors. The CH4 from fuel compressor at 30 bars enters the reactor. The reactor is fluidized bed for enhanced solid and gas mixing, heat transfer, mass transfer and reaction. The reaction in the fuel reactor is endothermic hence high temperature is preferred. The NiO stream coming from the air reactor is already at very high temperature because of exothermic reaction. This high temperature favors the endothermic reaction in fuel reactor. The reducing agent used here is CH4 as this is a combustion-based technique natural gas is used to reduce the NiO into Ni so that nitrogen production cycle continues. The CH4 itself oxidized, (combusts). The energy required to reduce NiO is greater than energy released by combustion of CH4 so overall this is an energy consumption reaction (endothermic reaction).

4.1.5 Heat Exchanger 1:

This heat exchanger is used to exchange heat between the NiO coming from the air reactor and the flue gases. As the flue gases are leaving the fuel reactor, which is endothermic, there temperature is quite low, to use this high-pressure flue gas for energy production, their temperature is increased by the heat exchanger. This heat exchanger is direct-contact, counter-current type. The solid particles flow from top to bottom, whereas gas rises in between it, as they are not miscible or mix, direct contact works better and has good efficiency for this type of heat exchange. By exchanging heat, the energy released in the exothermic reaction of air reactor is utilized for power generation via turbines.

4.1.6 Heat Exchanger 2:

In this heat exchanger the streams between which the heat is exchanged is the incoming fuel from the compressor and the outgoing stream of Ni (regenerated) in the fuel reactor. As the fuel coming from the compressor is at 185C and higher temperature is required for the endothermic reactor in fuel reactor, whereas Ni coming from the reactor is at 500C, lower temperature is required as this enters the air reactor which comprises of exothermic reactor and low temperature is favorable. So, to bring the reactants to the optimal conditions this heat exchanger is employed. The type of heat exchanger is direct contact type. The fuel passes through the bed of solids and is heated up.

4.1.7 Cyclone separator 1:

Is employed after the air reactor, as the fluidized bed reactor always have a cyclone separator at downstream because the stream leaving is always a mixture of solid and gas. Cyclone separator simply separates the solids and gas, the solid stream is dropped and flows through the bottom whereas the gaseous stream leaves from the top. The separation is based on the density difference of both species. The NiO stream leaves from the bottom whereas the N2 stream leaves the top.

4.1.8 Cyclone separator 2:

This separator is placed on the downstream of fuel reactor, this separated Ni and the flue gases. Separation is based on density difference.

4.1.9 N_2 Turbine:

High temperature and high pressure N_2 stream enters the turbine and is used to generate power. This gaseous stream rotates the turbine blades which produces shaft work and is used to generate electricity. The gas enters at 30 bars and exits at 5 bars from the turbines.

4.1.10 Gas Turbine:

High temperature and high-pressure flue gas enters the turbine and is used to generate power. This gaseous stream rotates the turbine blades which produces shaft work and is used to generate electricity. The gas enters at 30 bars and exits at 5 bars from the turbines. The flue gas on the downstream of gas turbine is exhaust gas, either it is released into the open atmosphere or sent to carbon capture unit.

4.1.11 Waste Heat Boiler:

Also known as heat recovery steam generator (HRSG) this boiler uses the waste flue gas which is at high temperature but low pressure enough to generate steam is known as waste heat boiler. The N_2 gas after downstream of turbine is at a very high temperature enough to generate steam.

4.1.12 Steam Turbine:

Steam Turbine is used to generate electricity and optimize the energy production process by using waste heat as well. The steam generated in waste heat boiler is used to generate electricity.

4.1.13 Condenser:

Condenser the steam at the downstream of turbine. As no moisture content should be present during the turbine operation as it is undesirable for the life of steam turbine. The physical state is saturated steam at downstream of gas turbine. As it is low pressure steam, it must regain high pressure for the turbine cycle again. For this it is first passed to the condenser. The steam condenses and becomes saturated liquid.

4.1.14 Pump:

The saturated liquid from the condenser passes to pump for high pressure.

4.2 Process Flow Diagram:

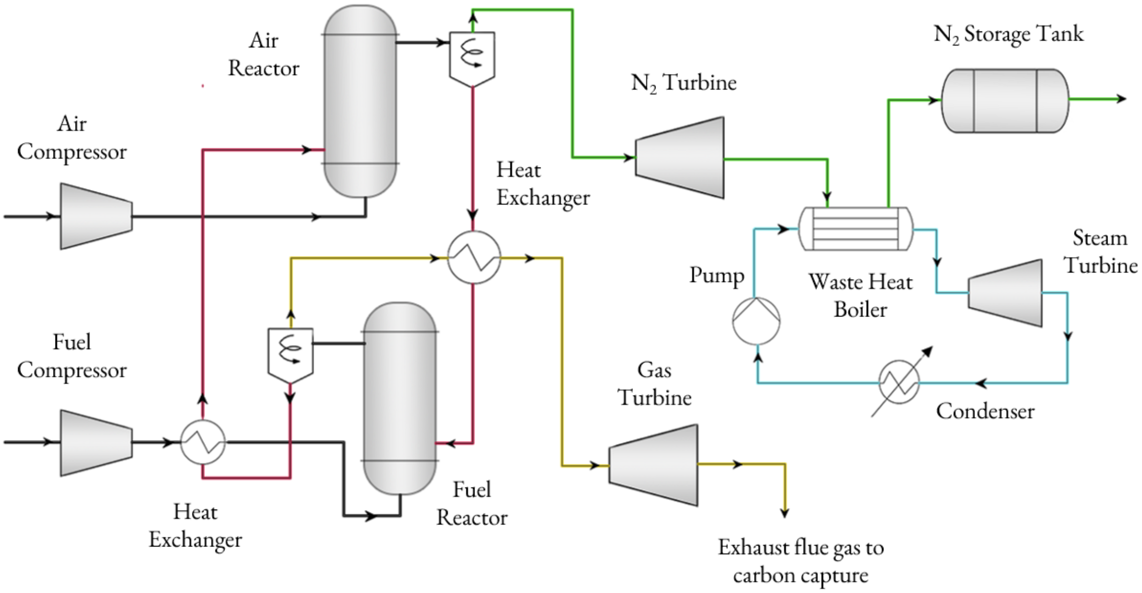


Figure 4.1 Process Flow Diagram

CHAPTER 5

MATERIAL BALANCE

5.1 Assumptions:

Material Balance involves the application of the law of conservation of mass to account for all the material that is entering and leaving a system. With the help of mass balance, the, flowrates and compositions of unknown streams can be calculated.

- FFC production = 1360 ton/day
- Nitrogen required = 5.6×10^3 kmol/hr (calculated from capacity).
- N_2 source is air as it contains 78 mol% N_2
- Assumptions for mass and energy balance is it's a steady state process.
- Basis = 1 hr.
- Pressure drops in the equipment are not considered.
- No material is lost.

5.2 Equation for mass balance:

- **Mass In – Mass Out + Generation – Consumption = Accumulation**
- Whereas for steady state accumulation, generation, consumption = 0
- **Mass In = Mass Out**
- Units = kmol/hr.

5.3 Air compressor:

- Composition of air: 78% N_2, 21% O_2, 1 % traces.
- Nitrogen required = 1.19×10^4 kg/hr (calculated from capacity).

Table 5.1 Mass Balance on Air compressor

Component	Inlet (kg/hr)	Outlet (kg/hr)
Total Air	2.1×10^5	2.1×10^5
N_2	1.57×10^5	1.57×10^5
O_2	0.5×10^5	0.5×10^5
Traces	0.02×10^5	0.02×10^5

5.4 Fuel Compressor:

Fuel assumed is purely methane. Amount of fuel entering is according to stoichiometric quantity required for complete combustion.

Table 5.2 Mass Balance on Fuel compressor

Component	Inlet (kg/hr)	Outlet (kg/hr)
CH_4	1.25×10^4	1.25×10^4

5.5 Air reactor:

Reaction: Oxidation reaction of Ni is very fast and shows the conversion of 99.6%.

$$4\text{Ni} + 2\text{O}_2 \rightarrow 4\text{NiO}; \quad \Delta\text{H} = -239.7\,\text{kJ/mol}$$

Table 5.3 Mass Balance on Air reactor

Component	Inlet (kg/hr)	Outlet (kg/hr)
N_2	1.57×10^5	1.57×10^5
O_2	0.5×10^5	0.002×10^5
Ni	1.81×10^5	0.007×10^3
NiO	-	3.09×10^3

5.6 Fuel reactor:

$$4\text{NiO} + \text{CH}_4 \rightarrow 4\text{Ni} + 2\text{H}_2\text{O} + \text{CO}_2; \quad \Delta H = 134.4\,\text{kJ/mol}$$

Side reaction is NiO + CH4 = CO + 2H2 + Ni (incomplete combustion)

Table 5.4 Mass Balance on Fuel reactor

Component	Inlet (kmol/hr)	Outlet (kmol/hr)
CH_4	0.78×10^3	-
Ni	0.0124×10^3	3.1×10^3
NiO	3.09×10^3	-
CO_2	-	0.73×10^3
H_2O	-	1.4×10^3
CO	-	0.04×10^3
H_2	-	0.12×10^3

5.6 Heat Exchanger – 01:

Heat exchangers are the devices which are used to exchange the heat between the two fluids. Energy balance was applied on the heat exchangers to calculate the heat exchanged between the two fluids. Energy released by the hot fluid must be exactly equal to the energy absorbed by the cold fluid. As the process is steady state, and no reaction, generation, accumulations take place within heat exchanger so **mass in = mass out.**

Table 5.5 Mass Balance on Heat exchanger-01

Component	Inlet (kg/hr)	Outlet (kg/hr)
Cold Stream		
CO_2	3.2×10^4	3.2×10^4
H_2O	2.52×10^4	2.52×10^4
CO	1.12×10^3	1.12×10^3
H_2	0.24×10^3	0.24×10^3
Hot Stream		
NiO	2.3×10^5	2.3×10^5

5.7 Heat Exchanger- 02:

As the process is steady state, and no reaction, generation, accumulations takes place within heat exchanger so **mass in = mass out.**

Table 5.6 Mass Balance on Heat Exchanger-02

Component	Inlet (kg/hr)	Outlet (kg/hr)
Cold Stream		
CH_4	1.25×10^4	1.25×10^4
Hot Stream		
Ni	1.82×10^5	1.82×10^5

5.8 Gas Turbine- 01:

As the process is steady state, and no reaction, generation, accumulations take place within heat exchanger so **mass in = mass out.**

Table 15.7 Mass Balance on Gas turbine-01

Component	Inlet (kg/hr)	Outlet (kg/hr)
N_2	1.57×10^5	1.57×10^5

5.9 Gas Turbine- 02:

As the process is steady state, and no reaction, generation, accumulations take place within turbine so **mass in = mass out.**

Table 5.8 Mass Balance on Gas Turbine-02

Component	Inlet (kg/hr)	Outlet (kg/hr)
CO_2	3.2×10^4	3.2×10^4
H_2O	2.52×10^4	2.52×10^4
CO	1.12×10^3	1.12×10^3
H_2	0.24×10^3	0.24×10^3
Total	5.86×10^4	5.86×10^4

5.10 Waste Heat Boiler:

As it is a steady and non-reactive process, hence mass in =mass out.

Table 5.9 Mass Balance on Waster heat boiler

Component	Inlet (kg/hr)	Outlet (kg/hr)
	Cold Stream	
Steam	2.4×10^4	2.4×10^4
	Hot Stream	
N_2	1.57×10^5	1.57×10^5

CHAPTER 6

ENERGY BALANCE

6.1 Assumptions:

Energy balance is done for the estimation of fuel, cooling media or energy requirements. Energy balance is also a key factor while designing the specifications of desire equipment. Following assumptions were made for the energy balance of the plant:

- The process is considered a steady state process which implies:
  $\Delta U + \Delta Ek + \Delta Ep = Q - Ws + W$
  $\Delta Ek = \Delta Ep = 0$
  $\Delta H = Q + W$

- For the energy balance of a component of a plant involving a reaction the following equation is used:
  $\Delta H_{r,t} = \Delta HP - \Delta HR + \Delta H_{reaction}$ (kJ/hr)
  Energy out= Energy in + generation - consumption

- The Enthalpy of each stream was calculated using the following formula
  $HT = m * \int Cp * dT$ (kJ /hr)

- To calculate the Cp of a mixed stream, containing more than one chemical species the following formula was used:
  Cp (mixture) = $xa\ Cp_a + xb\ Cp_b + xc\ Cp_c + \ldots\ldots\ldots\ldots$

6.2 Air compressor:

Polytropic work is considered in the compressor, as isentropic is an ideal phenomenon. Isentropic process states that the entropy remains constant during the compression and there is no heat transfer with the surrounding and system. Whereas practically, there is rise in temperature during compression and the compressor parts are heated up which shows this is not isentropic process. Considering polytropic work, following is the equation for calculation compressor work.

$$\mathbf{Ws} = \frac{\mathbf{ZRT_1}}{\mathbf{Mw}}\left(\frac{\mathbf{n}}{\mathbf{n-1}}\right)\left(\frac{\mathbf{P_2}}{\mathbf{P_1}}^{\frac{(\mathbf{n-1})}{\mathbf{n}}} - \mathbf{1}\right)$$

- Z = Compressibility factor
- R = Gas constant = 8.314 KJ/ Kmol K
- T_1 = Inlet temperature of the feed gas

The compression of air from 1 to 30 bar is done in **3 stages.** The pressure is divided such that each stage requires equal amount of work.

1st stage: 1- 3.11 bar

2nd stage: 3.11- 9.7 bar

3rd stage: 9.7- 30 bar

As: $\frac{P_2}{P_1} = \frac{P_3}{P_2} = \frac{P_4}{P_3}$ So, $\frac{3.11}{1} = \frac{9.7}{3.11} = \frac{30}{9.7} = \mathbf{3.11}$

- Values of Z and Cp/ Cv is taken from aspen hysys.
- Efficiency of compressor is taken from the following chart.
- Efficiency depends on volumetric flow rate.

Table 6.1 Energy Balance on Air compressor

Properties	**Energy balance on Air compressor**	
Stage 1	**Inlet**	**Outlet**
Pressure (bar)	1	3.11
Flow rate (kg/hr)	2.1 x 10^5	2.1 x 10^5
Avg Z factor	1.0002	
Avg Cp/ Cv	1.39	
Power Consumed	6.5 MW	
Stage 2		
Pressure (bar)	3.11	9.7
Avg Z factor	1.0004	
Avg Cp/ Cv	1.39	
Power Consumed	6.9 MW	
Stage 3		
Pressure (bar)	9.7	30
Avg Z factor	1.002	
Avg Cp/ Cv	1.41	
Power Consumed	6.9 MW	

Overall		
Pressure (bar)	1	30
Temperature (C)	25	185
Power consumed	**20.3 MW**	

6.3 Fuel compressor

$$\mathbf{Ws} = \frac{\mathbf{ZRT_1}}{\mathbf{Mw}}\left(\frac{\mathbf{n}}{\mathbf{n-1}}\right)\left(\frac{\mathbf{P_2}}{\mathbf{P_1}}^{\frac{(\mathbf{n-1})}{\mathbf{n}}} - \mathbf{1}\right)$$

- Z = Compressibility factor
- R = Gas constant = 8.314 KJ/ Kmol K
- T_1 = Inlet temperature of the feed gas

The compression of air from 1 to 30 bar is done in **2 stages.** The pressure is divided such that each stage requires equal amount of work.

- **1st stage: 1 - 5.5 bar**
- **2nd stage: 5.5 - 30 bar**

Table 6.2 Energy Balance on Fuel compressor

Properties	**Energy balance on Methane compressor**	
Stage 1	**Inlet**	**Outlet**
Pressure (bar)	1	5.5
Flow rate (kg/hr)	1.25×10^4	1.25×10^4
Avg Z factor	0.9981	
Avg Cp/ Cv	1.27	
Power Consumed	1.4 MW	
Stage 2		
Pressure (bar)	5.5	30
Avg Z factor	0.992	
Avg Cp/ Cv	1.28	
Power Consumed	1.4 MW	
Overall		
Pressure (bar)	1	30
Temperature (C)	25	187
Enthalpy (kJ/kmol)	900	7290
Density (kmol/m³)	0.04	0.79
Power consumed	**2.8 MW**	

6.4 Air reactor:

Energy balance on air reactor:

1) Calculating extent of reaction: Ɛ

$$Ɛ = \frac{(\dot{m}_{O2})_{out} - (\dot{m}_{O2})_{in}}{(V_{O2})}$$

$$Ɛ = \frac{(0.002 \times 10^5 - 0.5 \times 10^5)}{(-2)}$$

$$Ɛ = 24900 \text{ Kg/hr}$$

2) ΔH_r = Heat of reaction = -240kJ/mol (from literature)

3) Calculating inlet enthalpy: Reference temperature = 25°C

$$H_1 = \int_{25}^{450} Cp_{Ni} = \int_{25}^{450} 6.99 + 0.000905T = 21.38$$

$$H_2 = \int_{25}^{185} Cp_{O2} = \int_{25}^{185} 2.91 \times 10^{-3} + 1.158 \times 10^{-5} - 0.507 \times 10^{-8} = 5.3$$

$$H_3 = \int_{25}^{T} Cp_{NiO} = 11.3 + 0.00215T = \text{by solver}$$

$\Delta H = Ɛ\, H_r + \dot{m}_1 H_1 + \dot{m}_2 H_2 + \dot{m}_3 H_3 = 0$

$\Delta H = 0.0138T^2 + 170.64T - 220698$

T_{ad} = 1180°C (By solver)

Table 6.3 Energy Balance on Air reactor

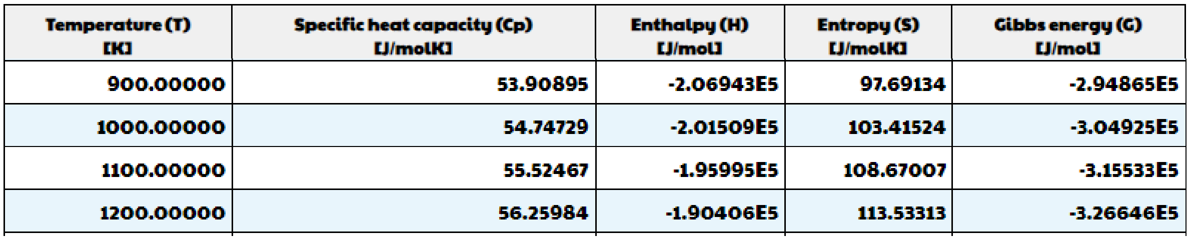
Properties	**Inlet**		**Outlet**	
	Air	**Ni**	**Air**	**NiO**
Temperature (˚C)	185	450	1180	1180
Pressure (bar)	30	-	30	-
Avg Cp (kJ/kg C)	3.2	0.55	0.4	
ΔH (˚kJ/kg)	0 (adiabatic reactor)			

6.5 Heat Exchanger- 01:

As there is no phase change while releasing or absorbing the energy in the fluids so no latent heat is involved. The equation used to calculate the energy released or absorbed is as follows:

Q = m Cp ΔT where m is the mass flow rate. Values for Cp are calculated from hysys.

$\Delta Hhot = - \Delta Hcold \qquad \Delta H_i = Q_i \qquad m_1\, Cp_1\, \Delta T_1 = - m_2\, Cp_2\, \Delta T_2$



Temperature (T) [K]	Specific heat capacity (Cp) [J/molK]	Enthalpy (H) [J/mol]	Entropy (S) [J/molK]	Gibbs energy (G) [J/mol]
900.00000	53.90895	-2.06943E5	97.69134	-2.94865E5
1000.00000	54.74729	-2.01509E5	103.41524	-3.04925E5
1100.00000	55.52467	-1.95995E5	108.67007	-3.15533E5
1200.00000	56.25984	-1.90406E5	113.53313	-3.26646E5

Figure 6.1 Cp values

- C_P of Hot Stream = 0.738 (kJ/kg C)
- C_P of cold Stream = 1.82 (kJ/kg C)

$Q = m_1C_{p1}\Delta T_{1} = m2Cp2\Delta T_2$

$= 5.87 \times 10^4$ kg/hr x 1.82 (kJ/kg C) x (390˚C) = (2.3×10^5 kg/hr) 0.738 x ΔT_2

$\Delta T_2 = 245.5$ ˚C

Table 6.4 Energy Balance on Heat excahnger-01

	Cold Stream		Hot Stream	
	Inlet	**Outlet**	**Inlet**	**Outlet**
Total mass flow (kg/hr)	5.87×10^4	5.87×10^4	2.3×10^5	2.3×10^5
Temperature (˚C)	500	720	1180	1043
Avg Cp (kJ/kg C)	1.82		0.738	
ΔT (˚C)	220		137	
Heat flow (kW)	6457		6457	

6.6 Heat Exchanger- 02:

As there is no phase change while releasing or absorbing the energy in the fluids so no latent heat is involved. The equation used to calculate the energy released or absorbed is as follows: **$Q = m\ Cp\ \Delta T$** where m is the mass flow rate.

$\Delta Hhot = - \Delta Hcold \qquad \Delta H_i = Q_i \qquad m_1\ Cp_1\ \Delta T_1 = - m_2\ Cp_2\ \Delta T_2$

Table 6.5 Energy Balance on Heat exchanger-02

	Cold Stream		**Hot Stream**	
	Inlet	**Outlet**	**Inlet**	**Outlet**
Total mass flow (kg/hr)	1.25×10^4	1.25×10^4	1.82×10^5	1.82×10^5
Temperature (˚C)	187	302	500	450
Avg Cp (kJ/kg C)	3.27		0.55	
ΔT (˚C)	115		50	
Heat flow (MW)	12.8		-12.8	

6.7 Gas Turbine- 01:

$$Ws = \frac{ZRT}{Mw}\frac{n}{(n-1)}\left(\frac{P_2}{P_1}^{\frac{(n-1)}{n}} - 1\right)$$

$$m = \frac{(\gamma - 1)}{\gamma} \times Ep \ \text{(For expansion)}$$

$$m = 0.177$$

Now finding value of n,

$$n = \frac{1}{1 - m}$$

$$n = 1.215$$

Table 6.6 Energy Balance on Gas turibne-01

Properties	**Inlet**	**Outlet**
Pressure (bar)	30	5
Flow rate (Kmol/hr)	1.57 x 10^5	1.57 x 10^5
Temperature (°C)	1180	764
Enthalpy (kJ/kg)	1417	862
Avg Cp/ Cv	1.32	
Avg Z factor	1.006	
Power Generated	21 MW	

6.8 Gas Turbine - 02:

$$\mathbf{Ws = \frac{ZRT}{Mw}\frac{n}{(n-1)}\left(\frac{P_2}{P_1}^{\frac{(n-1)}{n}} - 1\right)}$$

$m = 0.14$

$n = 1.16$

Table 6.7 Energy Balance on Gas turbine-02

Properties	**Inlet**	**Outlet**
Pressure (bar)	30	5
Flow rate (Kg/hr)	5.86×10^4	5.86×10^4
Temperature (˚C)	950	710
Enthalpy (kJ/kg)	1705.7	1166.4
Avg Cp/ Cv	1.23	
Avg Z factor	1.0	
Power Generated	7.5 MW	

6.9 Waste Heat Boiler:

- H_1 = 675.3 kJ/kg, enthalpy of water at 40 bar 151 ˚C (value taken from steam table).
- H_2 = 3558. kJ/kg, enthalpy of superheated at 40 bar 550 ˚C (value taken from steam table).
- **ΔH_{steam} = 2883 kJ/kg**

$Q = m\, Cp\, \Delta T = m\, \Delta H_{steam}$

Table 6.8 Energy Balance on Waste heat boiler

	Steam		**N_2**	
	Inlet	**Outlet**	**Inlet**	**Outlet**
Total mass flow (kg/hr)	2.4×10^4	2.4×10^4	1.57×10^5	1.57×10^5
Temperature (˚C)	151	550	710	514
Avg Cp (kJ/kg C)	2.3		1.17	
ΔT (˚C)	399		196	
Heat flow (kW)	6118		-6118	

6.10 Steam Turbine:

$$\mathbf{Ws = \frac{ZRT}{Mw}\frac{n}{(n-1)}\left(\frac{P_2}{P_1}^{\frac{(n-1)}{n}} - 1\right)}$$

$m = 0.17$

$n = 1.2$

Table 6.9 Energy Balance on Steam turbine

Component	Inlet (kg/hr)	Outlet (kg/hr)
H_2O	2.4×10^4	2.4×10^4
Temperature (˚C)	550	315
Pressure (bar)	40	5
Vapor fraction	1	1
Duty (MW)	3.1	

6.11 Condenser:

This equipment is used to condense water so that water is pumped to 40 bars. As pump cannot intake gases/ vapors. It's important to condense it. The steam is condensed by aid of cooling water.

- H_1 = 3110.11 kJ/kg, enthalpy of steam at 5 bar 315 ˚C (value taken from steam table).
- H_2 = 640.11 kJ/kg, enthalpy of saturated liquid at 5 bar 151 ˚C (value taken from steam table).
- **ΔH_{steam} = 2438 kJ/kg**

$Q = m\ Cp\ \Delta T = m\ \Delta H_{steam}$

$Q = m \times 0.4$ kJ/kg C x 15K = $(2.4 \times 10^4$ kg/hr) x (2438 kJ/kg)

m = 2.7×10^6 kg/hr of cooling water required.

Table 6.10 Energy Balance on Condenser

	Steam		**Cooling water**	
	Inlet	**Outlet**	**Inlet**	**Outlet**
Total mass flow (kg/hr)	2.4 x 10^4	2.4 x 10^4	9.7x 10^6	9.7x 10^6
Temperature (˚C)	315	151	20	35
Avg Cp (kJ/kg C)	3.2		0.4	
ΔT (˚C)	149		87.8	
Heat flow (kW)	-1.6 x 10^4		1.6 x 10^4	

6.12 Pump:

Pumps are used to increase the pressure of liquids. Following equation was used to calculate the duty of the pump:

$$\mathbf{W} = \frac{\dot{m}}{\boldsymbol{\eta}}\left(\frac{\boldsymbol{\Delta P}}{\rho}\right)$$

Where,

ṁ= mass flow rate kg/sec = 6.66 kg/sec

η= efficient =0.75

ΔP= pressure difference= (40-5) bar = 35 bar = 3.5 x 10^6 Pa.

ρ= density of fluid = 917 kg/m^3 at 5 bars 150˚C

$$W = \frac{6.66}{0.75}\left(\frac{3.5\ \text{x}10^6}{917}\right)$$

W = 34 kW

Table 6.10 Energy Balance on Pump

	Inlet	Outlet
Water mass flow (kg/hr)	2.4 x 10^4	2.4 x 10^4
Pressure (bar)	5	40
Temperature (˚C)	151	151
Avg density kg/m^3	917	
Pump duty (kW)	34	

CHAPTER 7

EQUIPMENT DESIGN

7.1 Fluidized Bed reactor:

Ni particles size = 600 microns or 0.6 mm

ε_{mf} = Bed void fraction at minimum fluidization velocity = 0.422

ρ_s= Solid density (Ni) = 8908 kg/m^3

ρ = Fluid density (air) = 18.89 kg/m^3

Φ_s sphericity = 0.95

U = viscosity of fluid (air) = 0.00003 N/m^2 s

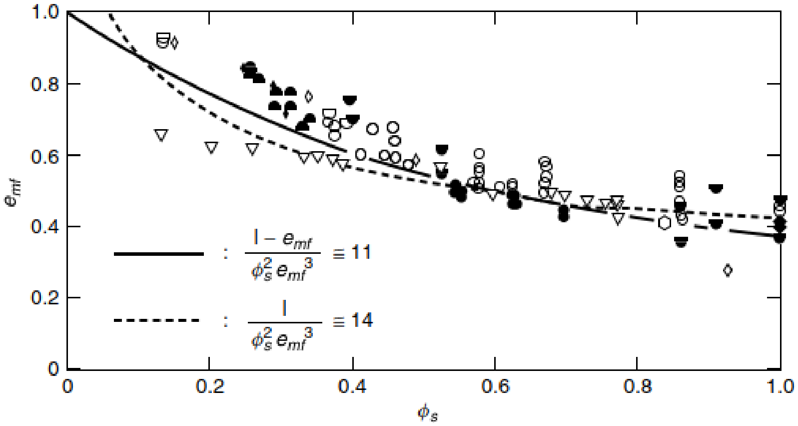


Figure 7.1 Relation between e_{mf} and $\emptyset_s$

Calculating Reynold's no. by following formula:

$$\frac{1.75}{\varepsilon_{mf}{}^3 \Phi s}(\mathrm{Re})^2 + \frac{150 -(1-\varepsilon_{mf})}{\varepsilon_{mf}{}^3 \Phi s^2}(\mathrm{Re}) = \frac{dp^3(\rho_s-\rho_g)}{u^2}$$

Solving quadratic equations:

$$= \frac{1.75}{(0.422)^3 0.95}(\mathrm{Re})^2 + \frac{150 - (1 - 0.422)}{(0.422)^3 (0.95)^2}(\mathrm{Re}) = \frac{0.02\times10^{-3}(18.89(8908-18.99))9.78}{0.00003^2}$$

$$= 24.86Re^2 + 2234.67\,Re - 14528 = 0$$

$\mathrm{Re} = 6.088$

Minimum fluidization velocity (U_{mf}):

$$\mathrm{Re} = \frac{\mathrm{dp}\ \mathrm{u_{mf}}\rho_g}{\mathrm{u}}$$

$U_{mf} = 0.048$ m/s

Terminal Velocity (u_t):

$$\mathrm{u_t} = \frac{\mathrm{dp}^2(\rho_s - \rho_g)\mathrm{g}}{18\mathrm{u}}$$

$u_t = 0.495\ m^2/s$

Diameter of Reactor:

$$\mathrm{dt} = \sqrt{\frac{4v_{or}}{u_{req}\pi}}$$

u_{req}= u_t =required velocity for fluidization that is terminal velocity in this case.

$$\mathrm{dt} = \sqrt{\frac{4(3.05)}{0.495\pi}}$$

$$\mathrm{dt} = 2.8$$

Diameter to height ratio D: H = 1:3

Reactor Height:

2.8m x 3 = 8.4 m

H = 8.4m

Pressure drop in Reactor:

Pressure drop equation: $\Delta P = (1 - e_{mf})(\rho_s - \rho) Lg$

Bed height (Lg) = 3.5 m

$e_{mf} = 0.422$

$g = 9.71\ ms^{-1}$

$\rho_{s,}\ \rho$ = already known

$\Delta P = 0.17$ bar

Table 7.1 Design of Fluidized bed reactor

Design specification of Fluidized Bed Reactor	
Reactor height	8.4 m
Reactor diameter	2.8 m
Pressure drop	0.17 bar
Terminal velocity	0.495 m/s
Air distributor	Perforated plate type

7.2 Cyclone Separator:

Inlet velocity (u) = 60 m/s

Nitrogen gas density (ρ) = 6.914 kg/m^3

Mass of N_2 = 1.91 x10^4 kg/hr

V = Volumetric flow rate of inlet air

$$V = \frac{1.91 \text{ x}104}{6.914 \times 3600} = 6.3 \text{ m}^3\text{/sec}$$

Area of the cyclone inlet duct formula: $A = \frac{\text{Inlet volumetric flow rate}}{\text{Inlet velocity}}$

$$A = \frac{6.3}{60} = 0.11 \text{ m}^2$$

Duct diameter (D_c) correlation: Area = $0.5D_c$ x $0.2D_c$

Area = 0.1 D_c^2

0.11 = 0.1 D_c^2

$$\sqrt{\frac{0.11}{0.1}} = D_c$$

D_c = 1.05m

Greater than 0.203m so, number of cyclone separator required:

$$\frac{1.05 \text{ m}}{0.203 \text{ m}} = 5 \text{ cyclones required}$$

Scaling factor = $\frac{d_2}{d_1}$

$=[(\frac{0.46}{0.203})^3 \times \left(\frac{223}{2.27\times10^4}\right) \times \left(\frac{0.065\times10^{-3}}{0.018\times10^{-3}}\right) \times \left(\frac{6718}{6713}\right)]^{0.5}$

$\sqrt{0.08} = 0.28$

D_c = 0.2 m, 5 cyclones are required

As 5 cyclones are required, hence flow rate = $\frac{6.3}{5} = 1.26$ m^3/ sec

New area = $\frac{1.26}{60} = 0.021$ m^2

D_c = 0.458 m ≈ 0.46

Correlations used to find other dimensions:

1. Inlet duct length = 0.46 m
2. Inlet duct width = 0.235 m
3. Length of chamber = 1.5D_c = 0.7
4. Length of cyclone = 2.5D_c = 1.15

Table 7.2 Design Specifications of Cyclone Separator

Design Specifications of cyclone separator	
Diameter of cyclone (D)	0.46 m
Length of chamber (H_1) = 1.5D_c	0.7 m
Length of cyclone (H_2) = 2.5D_c	1.15 m
Width of inlet (b) = 0.375D_c	0.1725 m

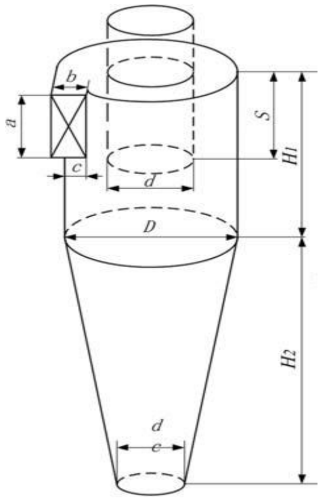


Figure 7.2 Cyclone Separator

7.3 Condenser (Shell & Tube):

Steam in = 100 ˚C, 1 bar (inlet)

Saturated liquid = 99.5 ˚C, 0.99 bar (outlet)

ΔT = 0.5 ˚C

Flow rate = 5.7×10^3 kg/hr

Enthalpy at inlet H_1 = 2676 KJ/kg

Enthalpy at outlet H_2 = 419 KJ/kg

ΔH = 2676-419 = 2257 KJ/kg

Total heat removed = $\dot{m}\Delta H$

= (5.7×10^3 kg/hr) (2257 KJ/kg) = 58344000 KJ/hr

= 3.6×10^3 kW = Heat load

Cooling water required = $m\Delta H = mC_p\Delta T$

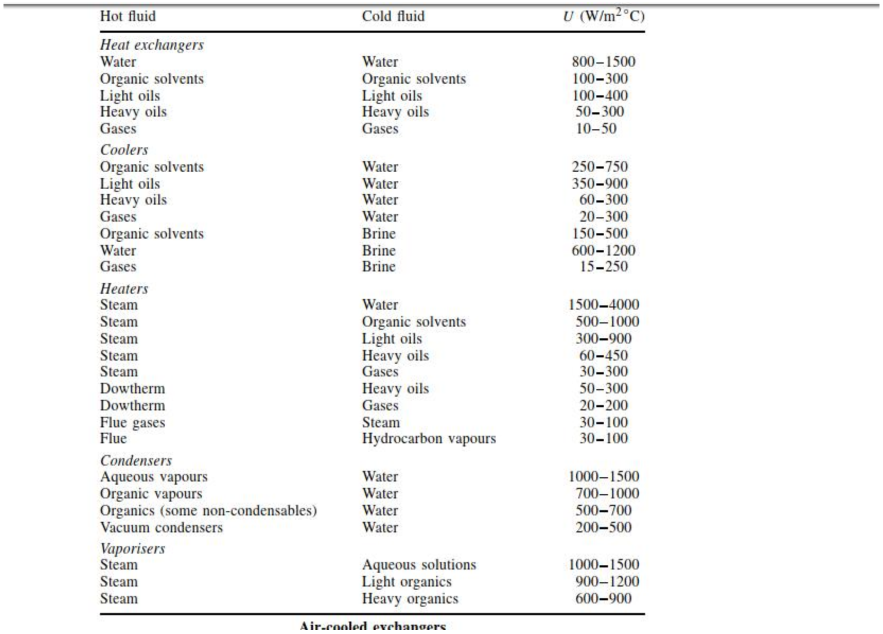
3.6×10^3 kg/sec = m x 4.18 x (40-25) = 55 kg/sec

$$\text{LMTD} = \frac{\Delta T_2 - \Delta T_1}{ln(\frac{\Delta T_2}{\Delta T_1})} = \frac{(100-40)-(99.5-25)}{ln(\frac{60}{74.5})}$$

LMTD = 67.49 ˚C

Heat Transfer area:

Assuming W = 1000 ˚CW^2/m ˚C



Hot fluid	Cold fluid	U (W/m^2°C)
Heat exchangers		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
Coolers		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
Heaters		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapours	30–100
Condensers		
Aqueous vapours	Water	1000–1500
Organic vapours	Water	700–1000
Organics (some non-condensables)	Water	500–700
Vacuum condensers	Water	200–500
Vaporisers		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Air-cooled exchangers

Figure 7.3 Design of Condenser

$\Delta T = 0.5$ °C, u = 1000 w/m^2 C, Q = 3.6 x10^3 kW

Q = (Area) (u) (ΔT)

$$A = \frac{3.6\times10^3}{(1000)(0.5)} \times 1000$$

A = 142 m^2 (trial area)

FT correction factor:

$$R = \frac{\Delta T_{hot}}{\Delta T_{cold}} = \frac{0.5\ ^{\circ}C}{15\ ^{\circ}C} = 6.2$$

$$S = \frac{\Delta T_{cold}}{T_2 - T_1} = \frac{15\ ^{\circ}C}{100^{\circ}C - 25^{\circ}C} = 0.09$$

$F_T = 0.97$

Mean Temperature = $F_{T\ (factor)}$ x LMTD = 0.97 x 67.49 °C = 65 °C

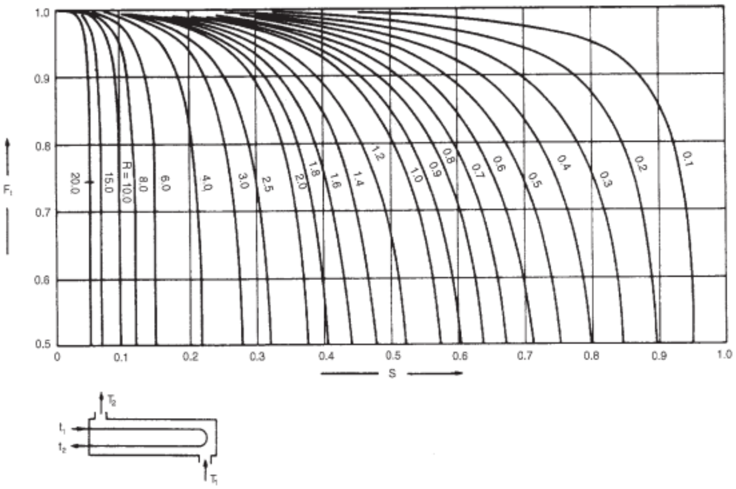


Figure 7.4 FT Correction Factor

Tubes Assumptions:

Outer diameter = 20mm

Inner diameter = 16.8mm

Length = 4.88m

Area = 2πrL

= π x 20 x 10^{-3} x 4.88 2r = diameter

= 0.3066

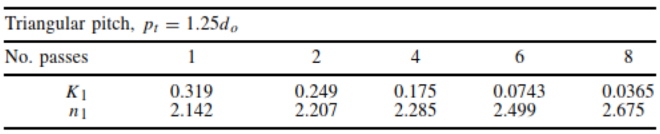
No. of tubes =$\frac{HT\ area}{Tubes\ area} = \frac{172}{0.3066}$

No. of tubes = 561

Pitch type = triangular factor = 1.25

Tubes bundle diameter:

1.25 x 20mm =25 mm (1 shell pass, 2 shell passes, triangular pitch)



Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675

Figure 7.5 Pitch

$D_b = 20(\frac{561}{0.249})^{\frac{1}{2.207}}$

D_b = 660 mm = 0.66 m

Shell side coefficient:

Mean temp shell side: $\frac{100+99.5}{2} = 99.75\ ^\circ C$

Mean temp tube side: $\frac{40+25}{2} = 32.5\ ^\circ C$

$(99.75 - T_w)\ 4000 = (99.75\text{-}32.5)1000$

Assuming 4000 $W/m^2.\ ^\circ C$ as condensing coefficient for steam.

T_w = tube wall assumed temperature = 116 °C

Physical properties at 116 °C:

1. ρ_L = 944.28 kg/m^3 (steam table)
2. μ_L = 0.8 C_p (mPa.s)
3. k_L = 0.48 W/m°C
4. ρ_V = 1.056 kg/m^3
5. Th = $\frac{Wc}{LNt} = \frac{2.4 \times 10^4}{4.88 \times 561} = 2.4 \times 10^{-3}$ kg/ms
6. No. of tubes in center row

   Nr = $\frac{D_b}{Pt} 1 = \frac{660}{25} = 27$

   Nr = $\frac{2}{3} \times (27) = 18$

Calculating coefficient: shell side

$h = 0.95 \text{ x } K_L \text{ x } [\frac{944(\rho_L - \rho_g)g}{\mu \times Th}]^{\frac{1}{3}} \times Nr^{\frac{-1}{6}}$

$h = 0.95 \text{ x } 0.48 \text{ x } [\frac{944(944-1.056)9.81}{0.8 \times 10^{-3} \times 2.435 \times 10^{-3}}]^{\frac{1}{3}} \times 18^{\frac{-1}{6}}$

h= 4647, which is close to assumed value

Tube side coefficient:

Cross sectional area of tubes = $\frac{\pi}{4} d^2\ or\ \pi r^2$

$= \frac{\pi}{4}(16.8 \times 10^{-3})^2$

$= 2.2 \times 10^{-4}\ m^2$

As tube pass = 2

Total no. of tubes = 561

Tubes per pass = 561/2 = 280.5

Total per pass tube area = $2.2 \times 10^{-4}\ m^2 \times 280.5 = 0.06\ m^2$

Avg tube side temp (in & out of cooling water)

T = $\frac{25+40}{2}$ = 32.5 ˚C

- ρ of water at 32.5 ˚C = 993 kg/m^3
- Flow rate of cooling water = 255 kg/s

Tube Velocity = $\frac{255\ \text{kg/sec}}{993\ \text{kg/m3}} \times \frac{1}{0.06\ \text{m2}} = 4.28\ \text{m/s}$

Tube velocity = 4.28 m/s

Tube side coefficient:

Following equation is used to find equation of water,

$$h = \frac{4200(\ 1.35 + 0.02t)u_t^{0.8}}{d_i^{0.2}}$$

Where,

d_i = tube inside diameter

t = water temperature (avg)

u_t = water velocity

$$h = \frac{4200(\ 1.35 + 0.02(32.5\ ^\circ\mathrm{C}))4.27^{0.8}}{(16.8\ \times 10^{-3})^{0.2}}$$

$$h = 5671\mathrm{W/m^\circ C}$$

Fouling factor assume = 6000 W/m^2 °C

Kw = 50 W/m°C

Calculating overall coefficient:

$$\frac{1}{u} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \times \ln\left(\frac{d_o}{d_i}\right)}{2kw} + \left[\frac{d_o}{d_i} \times \frac{1}{h_{id}}\right] + \left[\frac{d_o}{d_i} \times \frac{1}{h_i}\right]$$

$$\frac{1}{u} = \frac{1}{4647} + \frac{1}{6000} + \frac{20 \times 10^{-3} \times \ln\left(\frac{20}{16.8}\right)}{2 \times 50} + \left[\frac{20}{16.8} \times \frac{1}{6000}\right] + \left[\frac{20}{16.8} \times \frac{1}{5671}\right]$$

$$u = 1100\ \mathrm{w/m^2 {}^\circ C}$$

Which is close to assumed value of 1000 W/m^2 °C

Shell side pressure drop:

Assumptions, baffle spacing = shell diameter, 45 %

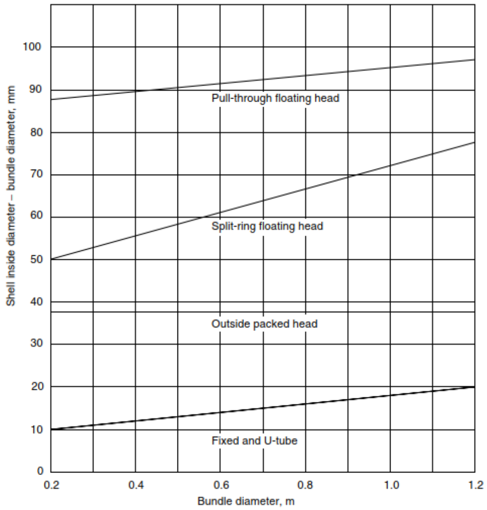


Figure 7.6 Shell inside diameter vs shell bundle clearance

- Clearance =95 mm

- Shell internal dia = 1035 + 95 = 1130 mm

- Cross flow area = $\frac{(\mathrm{pt}-\mathrm{d_o})\mathrm{D_s L_B}}{\mathrm{pt}}$ where,

Pt = tube pitch

d_o = tube outside dia

D_s = shell inside dia

L_b = baffle spacing

Cross flow area = $\frac{(25-20)\times1130\times1130\times10^{-6}}{25}$ = 0.255 m^2

Mass flow rate in shell = $(\frac{2.4\times10^4}{3600})\times\left(\frac{1}{0.255}\right) = 26.14\,\mathrm{kg/m^2s}$

Equivalent diameter d_e

$$\mathrm{d_e} = \frac{1.10}{\mathrm{d_o}}(\mathrm{pt}^2 - 0.917\mathrm{d_o}^2)$$

$$\mathrm{d_e} = \frac{1.10}{20}(25 - 0.917 \times 20^2)$$

$$\mathrm{d_e} = 14.201\ \mathrm{mm}$$

Vapor viscosity = 1.4 x10^{-2} mNs/m^2 = 1.4 x10^{-5} Pa. s

$\mathrm{Re} = \frac{\mathrm{G_s}\times\mathrm{d_e}}{\mathrm{u_{vapor}}}$

$\mathrm{Re} = \frac{26.14\times14\times10^{-3}}{1.4\times10^{-5}}$

$\mathrm{Re} = 26140$

From figure 12.30, jf = 4.2 x10^{-2}

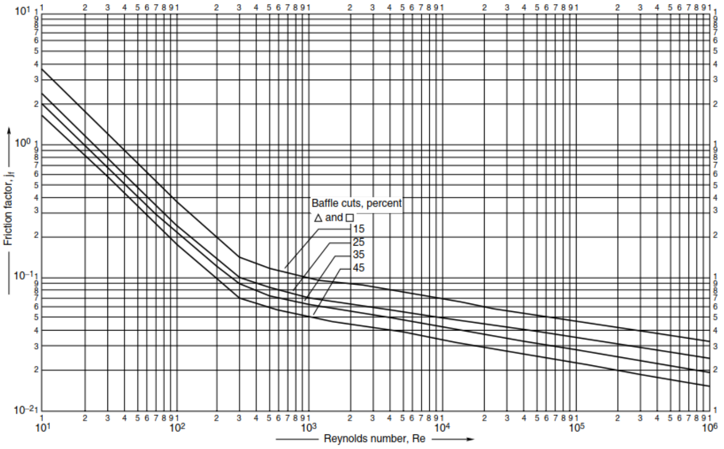


Figure 7.7 Friction Factor vs Reynolds number

Velocity shell side,

Velocity $=\frac{\mathrm{Gs}}{\rho_v} = \frac{26.14}{1.05} = 24.89\ \mathrm{m/s}$

Pressure drop,

Equation for ΔP is:

$$\Delta P_{shell} = 8 j_f \left(\frac{D_s}{d_e}\right)\left(\frac{L}{L_b}\right)\left(\frac{\rho {U_s}^2}{2}\right)\left(\frac{u}{u_w}\right)^{-0.14}$$

$$\Delta P_{shell} = 8(4.2 \times 10^{-2})\left(\frac{1130}{14.2}\right)\left(\frac{4.88}{1.130}\right)\left(\frac{1.05 \times 24.89^2}{2}\right)\left(\frac{u}{u_w}\right)^{-0.14}$$

$$\Delta P_{shell} = 7234\ \mathrm{N/m^2}$$

$$\Delta P_{shell} = 0.07\ \mathrm{bar}$$

Tube side pressure drop:

Viscosity of water (cooling water):

$$\mathrm{Re} = \frac{U_t \rho d_i}{u} = \frac{4.28 \times 993 \times 16.8 \times 10^{-3}}{0.6 \times 10^{-3}}$$

$\mathrm{Re} = 119001$

U_t = velocity

u = viscosity

ρ = water density

d_i = tube inside dia

Calculating j_f factor from figure:

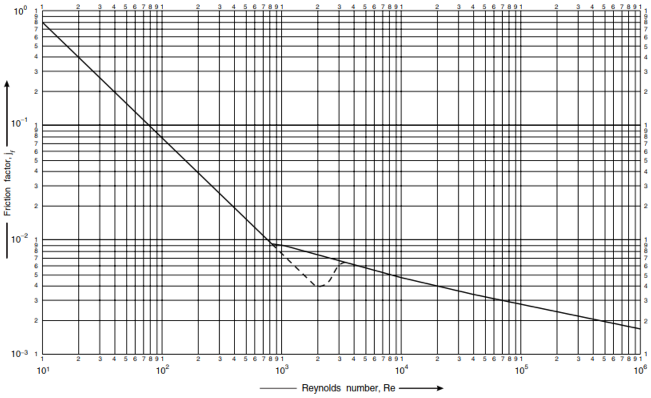


Figure 7.8 Friction Factor vs Reynolds number

$J_f = 2.9 \text{ x} 10^{-3}$

$$\Delta P = 2\left[8 j_f \left(\frac{L}{d_i}\right) + 2.5\right] \times \frac{\rho U_t}{2}$$

$$\Delta P = 2\left[8 \times 2.9 \times 10^{-2}\left(\frac{4.88}{16.8 \times 10^{-3}}\right) + 2.5\right] \times \frac{993 \times 4.28}{2}$$

$\Delta P = 54 \text{ kPa} = 7.25 \text{ psi}$, acceptable tube side ΔP

Table 7.3 Design Specifications of Condenser

Parameter	Value
Duty (kW)	$3.6 \text{ x} 10^3$

LMTD (˚C)	67.49	
Cooling water required (kg/sec)	55	
Heat Transfer Area (m^2)	142	
FT Correction factor (FT)	0.97	
Tubes Area (m^2)	0.3066	
Coefficient (W/m˚C)	4647 (Shell side)	5671 (Tube side)
Overall Co-efficient (W/m^2°C)	1100	
Equivalent diameter d_e (m)	0.014201	
Velocity (m/s)	24.89	-
Pressure Drop (bar)	0.07 (shell side)	0.54 (Tube side)

CHAPTER 8

SIMULATION

8.1 Simulation Tool:

Aspen HYSYS simulation software is used for the simulation as it contains the necessary equation of state, fluid package and equipments for the simulation of nitrogen production based on combustion technology.

As we know that the world is shifting towards Artificial Intelligence, so the need for simulation software has become significantly important. Aspen HYSYS simulation software is one of the best software for the modelling and simulation of process industries because of the following reasons:

1. **Prediction and Analysis:** It allows for the creation of virtual models that mimic real- world systems or processes. By running simulations, we can predict and analyze the behavior of these systems before implementing them in the physical world.

2. **Cost and Time Savings:** Simulating complex systems or processes can save significant costs and time compared to physical prototyping and testing.

3. **Design and Optimization:** It enables engineers and designers to create virtual prototypes and test different design iterations. This iterative process helps in optimizing designs and improving product quality.

4. **Performance Evaluation**: It allows us to evaluate and compare the performance of different systems or processes under various conditions. It can help optimize manufacturing processes.

5. **Visualization and Communication:** It often provides visual representations of complex data and models, making it easier to understand and communicate findings.

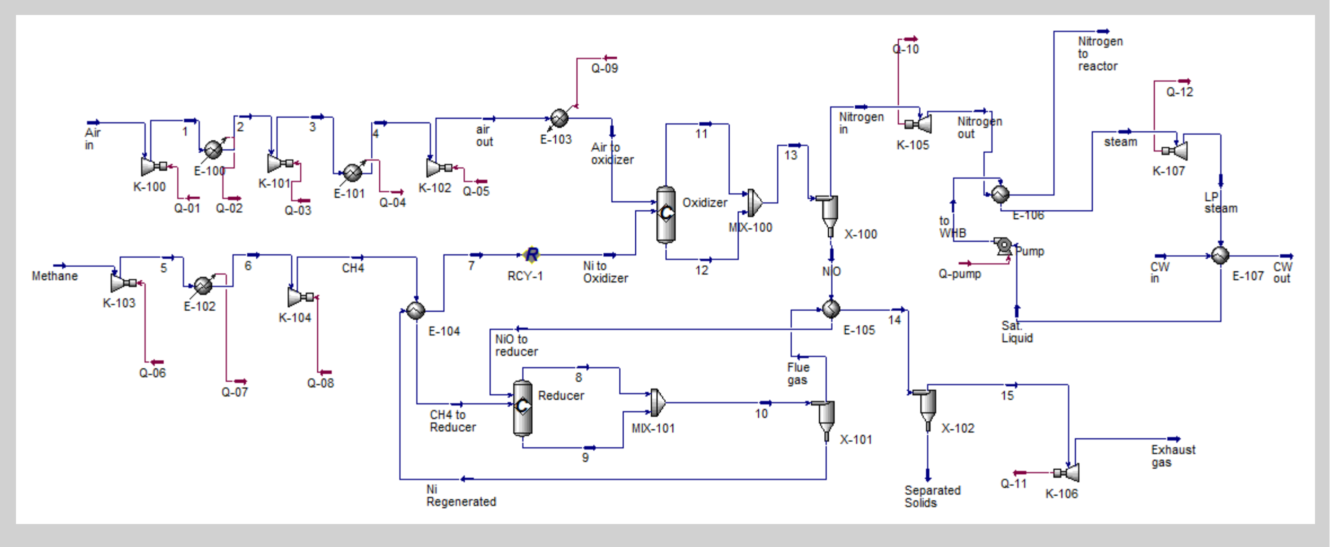
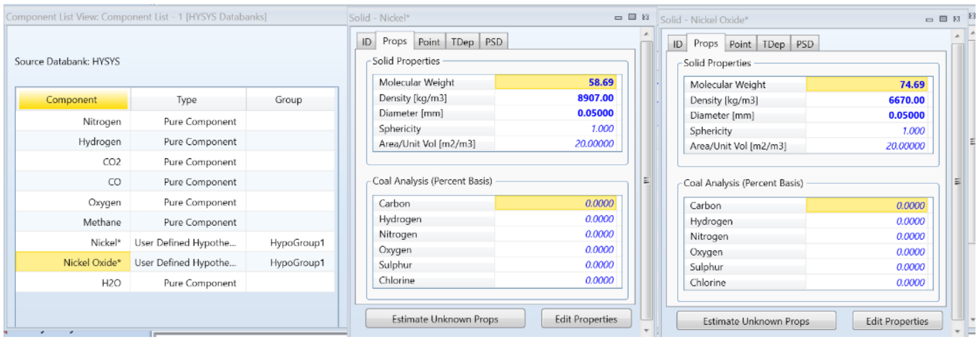


Figure 8.1 Overall Simulation process

8.2 Components:

The following components were selected from the component list of aspen HYSYS, The solids employed in this process are user defined. To enable the solids the following specifications were defined. (Particle size of solids is considered as 0.05mm):

1. Specific Capacity
2. Particle Size
3. Solid density
4. Molecular weight
5. Heat of formation



Source Databank: HYSYS

Component	Type	Group
Nitrogen	Pure Component	
Hydrogen	Pure Component	
CO2	Pure Component	
CO	Pure Component	
Oxygen	Pure Component	
Methane	Pure Component	
Nickel*	User Defined Hypothe...	HypoGroup1
Nickel Oxide*	User Defined Hypothe...	HypoGroup1
H2O	Pure Component	

Solid - Nickel*

Solid Properties

Molecular Weight	58.69
Density [kg/m3]	8907.00
Diameter [mm]	0.05000
Sphericity	1.000
Area/Unit Vol [m2/m3]	20.00000

Coal Analysis (Percent Basis)

Carbon	0.0000
Hydrogen	0.0000
Nitrogen	0.0000
Oxygen	0.0000
Sulphur	0.0000
Chlorine	0.0000

Solid - Nickel Oxide*

Solid Properties

Molecular Weight	74.69
Density [kg/m3]	6670.00
Diameter [mm]	0.05000
Sphericity	1.000
Area/Unit Vol [m2/m3]	20.00000

Coal Analysis (Percent Basis)

Carbon	0.0000
Hydrogen	0.0000
Nitrogen	0.0000
Oxygen	0.0000
Sulphur	0.0000
Chlorine	0.0000

Figure 8.2 Component List

8.3 Fluid Package:

The fluid package selected for this process simulation is Peng- Robinson. The Peng-Robinson equation of state (PR EOS) is widely used in process simulation for several reasons:

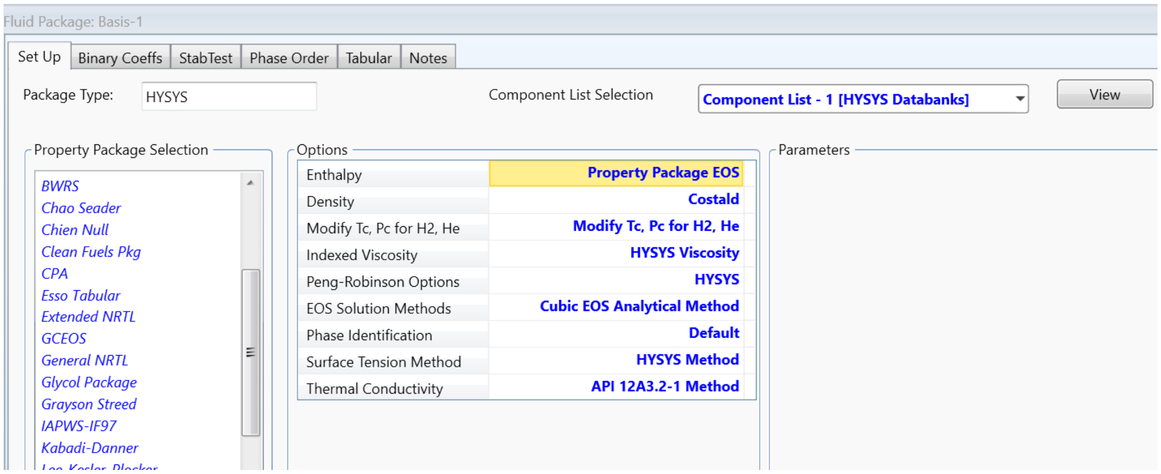
1. Accuracy: PR EOS provides reasonably accurate predictions of the thermodynamic properties of fluids over a wide range of temperature and pressure conditions, making it suitable for various industrial processes.

2. Versatility: It can handle a variety of fluid types, including hydrocarbons, pure components, polar compounds, and mixtures, which are commonly encountered in process industries such as oil and gas, chemical engineering, and pharmaceuticals.

3. Phase Behavior: PR EOS accurately predicts phase behavior, including vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE), critical points, and compressibility factors. This makes it valuable for simulating separation processes, distillation, and other unit operations.

5. Widely Accepted: It is one of the most widely accepted and validated equations of state, with extensive experimental data available for parameter estimation and validation, ensuring its reliability in process simulation.

Overall, the combination of accuracy, versatility, simplicity, and widespread acceptance makes the Peng-Robinson equation of state a popular choice for process simulation across various industries.



Package Type: HYSYS

Component List Selection: Component List - 1 [HYSYS Databanks]

Enthalpy	Property Package EOS
Density	Costald
Modify Tc, Pc for H2, He	Modify Tc, Pc for H2, He
Indexed Viscosity	HYSYS Viscosity
Peng-Robinson Options	HYSYS
EOS Solution Methods	Cubic EOS Analytical Method
Phase Identification	Default
Surface Tension Method	HYSYS Method
Thermal Conductivity	API 12A3.2-1 Method

Figure 8.3 Fluid Package

8.4 Reaction set:

Two reaction sets are defined for oxidizer and reducer each. Conversion reactions are chosen as the mass balance is based on the conversion of the reaction. The reactions are attached to the fluid package. Set -1 consists of one reaction, whereas reaction. Set-2 consists of two reactions with following conversions:

Reaction set – 01:

$2O_2 + 4Ni \rightarrow 4NiO$

$\Delta H = -239.7$ kJ/mol

Conversion = 99.7%

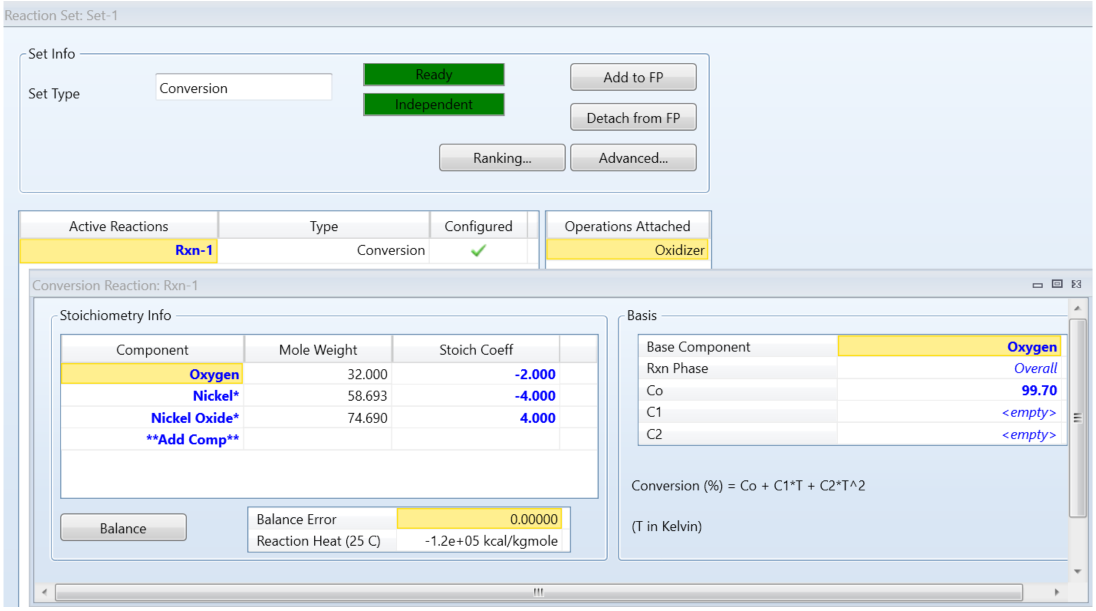
Reaction set – 02:

$4NiO \rightarrow 4Ni + 2O_2$

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

$\Delta H = +134.4$ kJ/mol

Conversion = 100% (complete combustion assumed)



Reaction Set: Set-1

Set Info

Set Type: Conversion

Ready

Independent

Active Reactions	Type	Configured
Rxn-1	Conversion	✓

Operations Attached
Oxidizer

Conversion Reaction: Rxn-1

Stoichiometry Info

Component	Mole Weight	Stoich Coeff
Oxygen	32.000	-2.000
Nickel*	58.693	-4.000
Nickel Oxide*	74.690	4.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-1.2e+05 kcal/kgmole

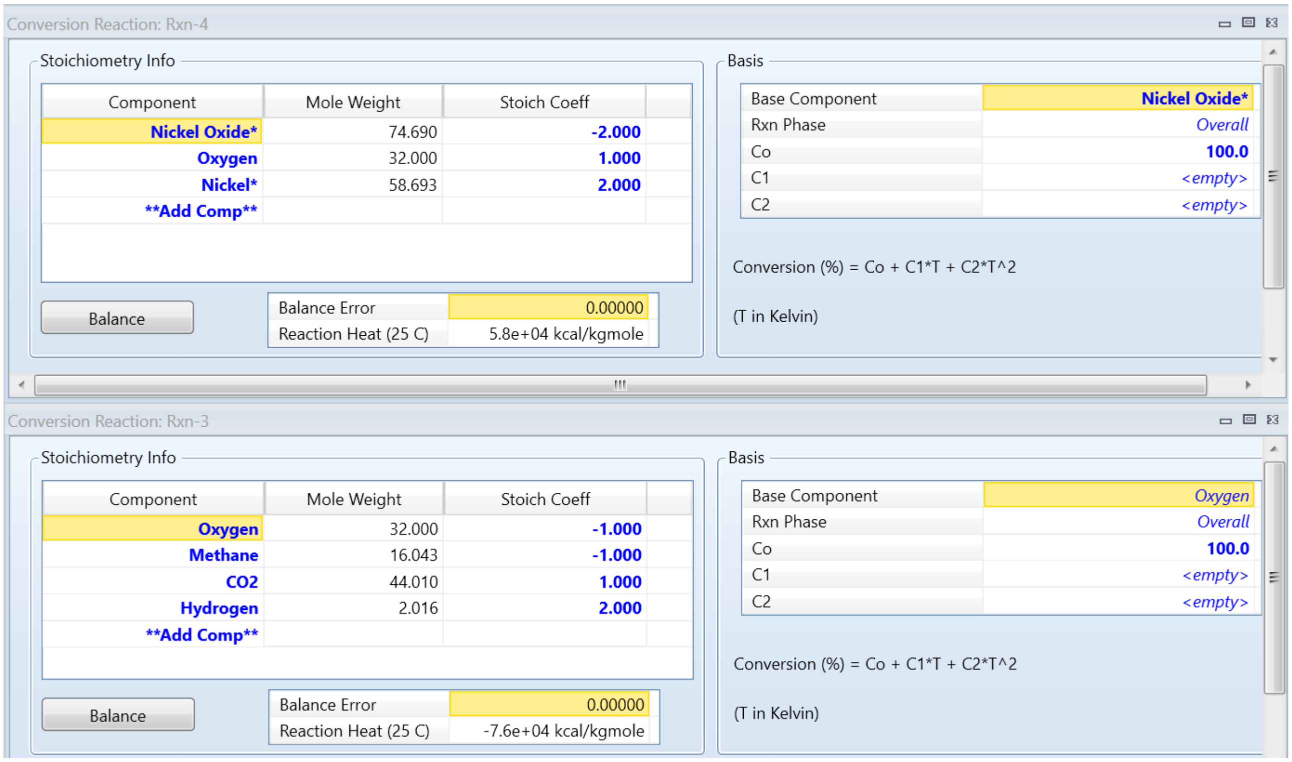
Basis

Base Component	Oxygen
Rxn Phase	Overall
Co	99.70
C1	<empty>
C2	<empty>

Conversion (%) = Co + C1*T + C2*T^2

(T in Kelvin)

Figure 8.4 Reaction Set 1



Component	Mole Weight	Stoich Coeff
Nickel Oxide*	74.690	**-2.000**
Oxygen	32.000	**1.000**
Nickel*	58.693	**2.000**
****Add Comp****		

Balance Error	0.00000
Reaction Heat (25 C)	5.8e+04 kcal/kgmole

Base Component	**Nickel Oxide***
Rxn Phase	*Overall*
Co	**100.0**
C1	*<empty>*
C2	*<empty>*

Conversion (%) = Co + C1*T + C2*T^2

(T in Kelvin)

Component	Mole Weight	Stoich Coeff
Oxygen	32.000	**-1.000**
Methane	16.043	**-1.000**
CO2	44.010	**1.000**
Hydrogen	2.016	**2.000**
****Add Comp****		

Balance Error	0.00000
Reaction Heat (25 C)	-7.6e+04 kcal/kgmole

Base Component	*Oxygen*
Rxn Phase	*Overall*
Co	**100.0**
C1	*<empty>*
C2	*<empty>*

Conversion (%) = Co + C1*T + C2*T^2

(T in Kelvin)

Figure 8.5 Reaction type

8.5 Simulation environment:

After the components, fluid package and reaction set have been selected, the software is not ready to simulate the process. For this model pallet is used to select the equipments e.g. compressors, coolers, heat exchangers etc. to obtain the results and simulate the process.

8.6 Multistage Compressors:

Multistage compressors are employed for two streams, air and fuel (methane). These compressors are employed with intercoolers as compression increases the temperature of the gaseous streams. These intercoolers decrease the temperature of the stream along with increasing pressure by compressors. 3 compressors with 2 intercoolers are employed for air stream whereas 2 compressors with 1 intercooler for fuel. Following is the worksheet and specs entered for converging and simulating compressors.

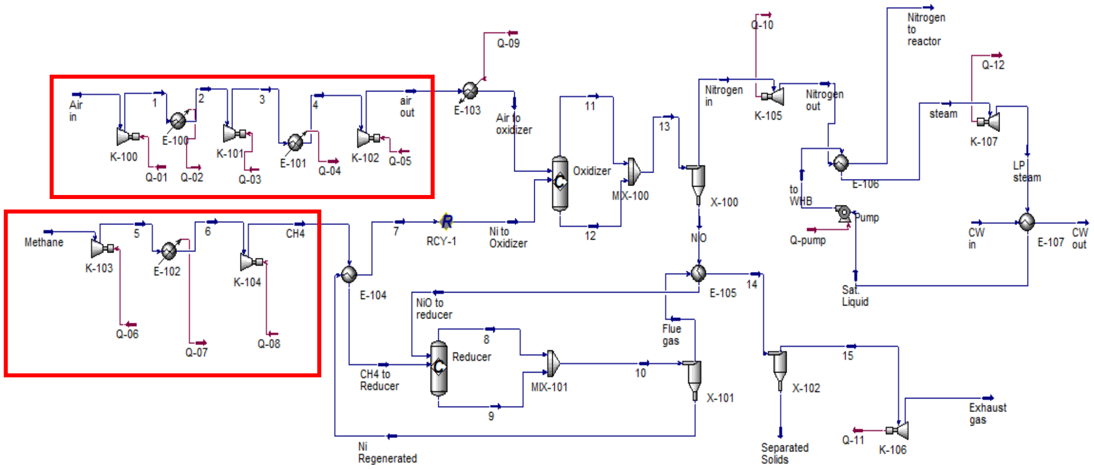
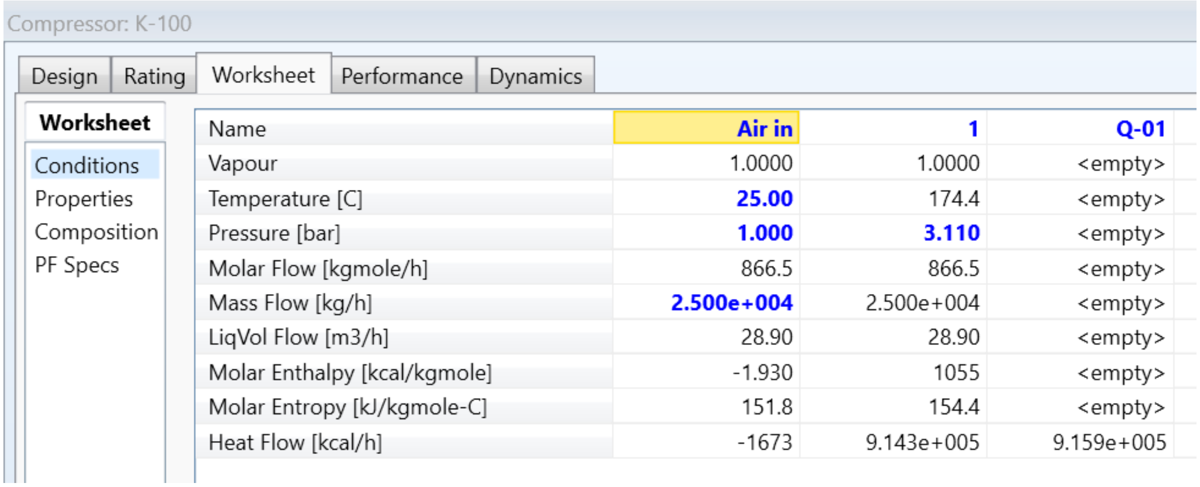
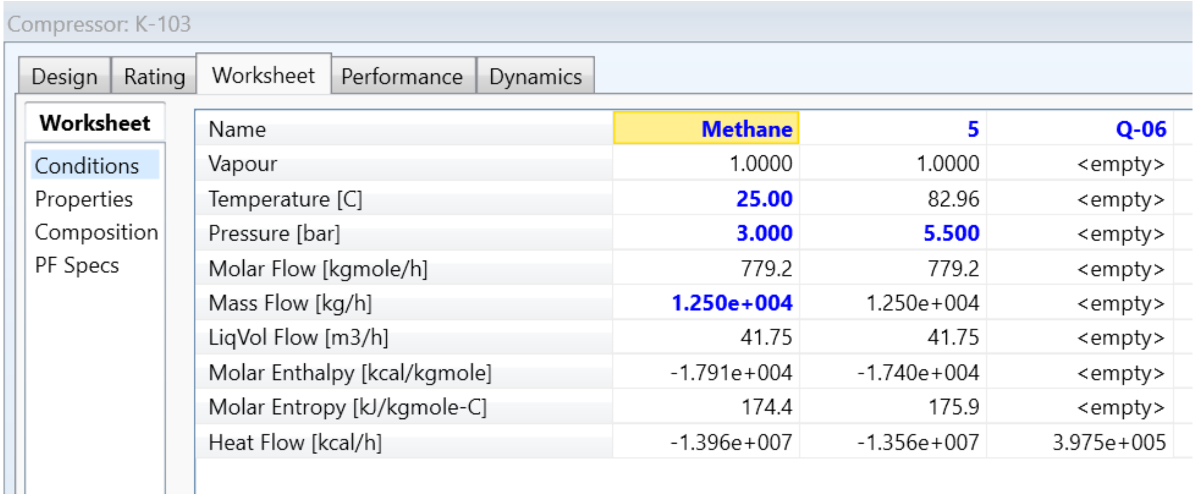


Figure 8.6 Multistage compressors



Name	Air in	1	Q-01
Vapour	1.0000	1.0000	<empty>
Temperature [C]	25.00	174.4	<empty>
Pressure [bar]	1.000	3.110	<empty>
Molar Flow [kgmole/h]	866.5	866.5	<empty>
Mass Flow [kg/h]	2.500e+004	2.500e+004	<empty>
LiqVol Flow [m3/h]	28.90	28.90	<empty>
Molar Enthalpy [kcal/kgmole]	-1.930	1055	<empty>
Molar Entropy [kJ/kgmole-C]	151.8	154.4	<empty>
Heat Flow [kcal/h]	-1673	9.143e+005	9.159e+005

Figure 8.8 Compressor 2 conditions



Name	Methane	5	Q-06
Vapour	1.0000	1.0000	<empty>
Temperature [C]	25.00	82.96	<empty>
Pressure [bar]	3.000	5.500	<empty>
Molar Flow [kgmole/h]	779.2	779.2	<empty>
Mass Flow [kg/h]	1.250e+004	1.250e+004	<empty>
LiqVol Flow [m3/h]	41.75	41.75	<empty>
Molar Enthalpy [kcal/kgmole]	-1.791e+004	-1.740e+004	<empty>
Molar Entropy [kJ/kgmole-C]	174.4	175.9	<empty>
Heat Flow [kcal/h]	-1.396e+007	-1.356e+007	3.975e+005

Figure 8.7 Compressor 1 conditions

8.7 Reactors:

Two reactors, Oxidizer and reducer also called air reactor and fuel reactor respectively are employed for the reaction. The reaction set – 01 is selected for oxidizer whereas reaction set - 02 is selected for the reducer. Ni reacts with O2 in air and oxidizes in the oxidizer, whereas NiO is reduced to Ni by reacting with methane. Methane is the reducing agent, itself oxidizes (combustion), regenerating the Ni which is continuously circulating in the fluidized bed reactors. Conversion reactor is selected for these reactors as the reaction set is conversion. Reaction – 01 completed 99.7%, whereas reaction – 02 completed 100%. The composition of the streams in and out of reactor shows the reaction has took place.

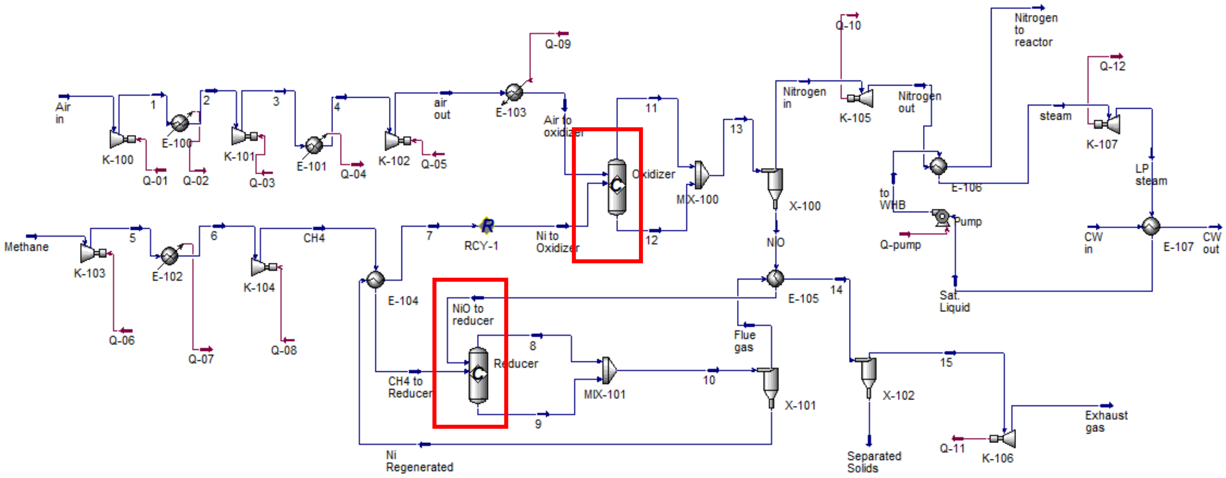
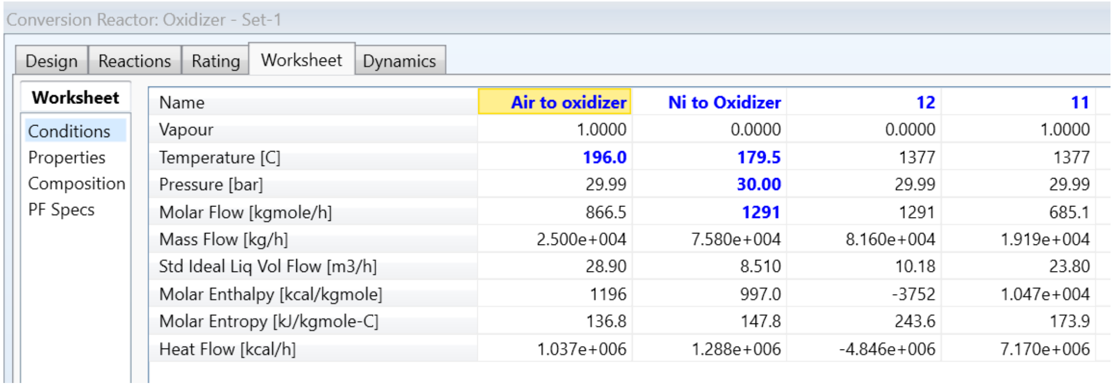
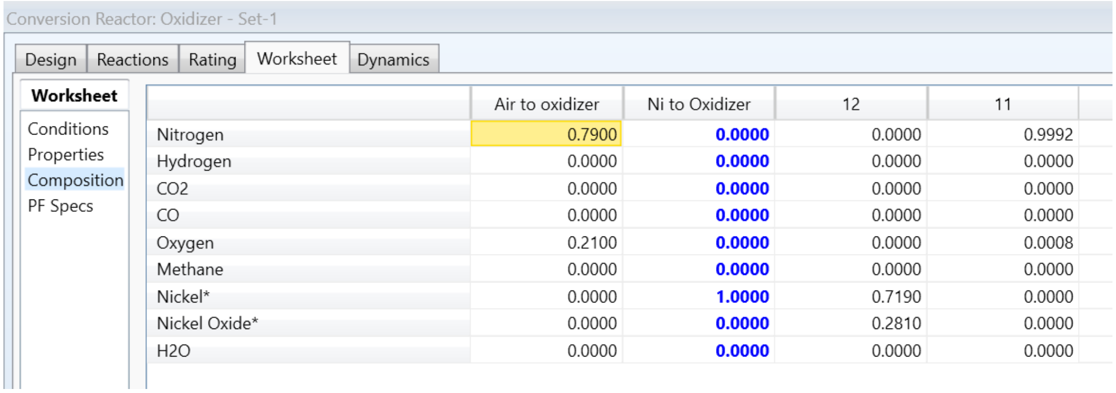


Figure 8.9 Reactors



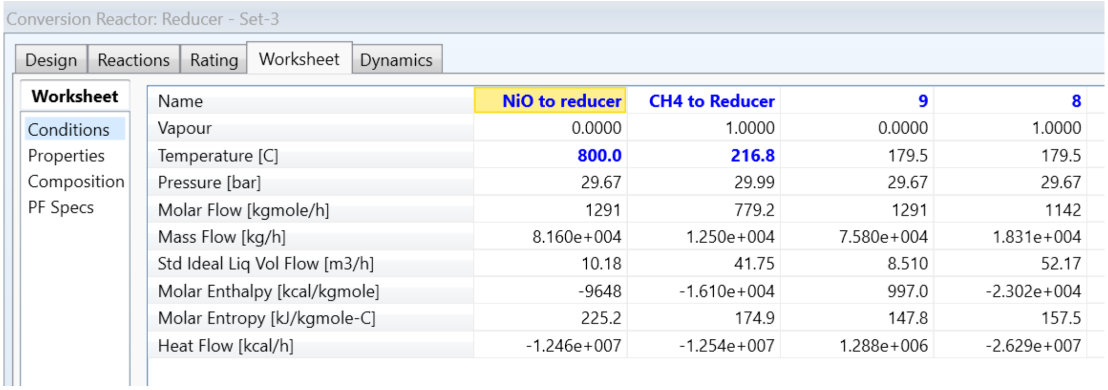
Name	Air to oxidizer	Ni to Oxidizer	12	11
Vapour	1.0000	0.0000	0.0000	1.0000
Temperature [C]	196.0	179.5	1377	1377
Pressure [bar]	29.99	30.00	29.99	29.99
Molar Flow [kgmole/h]	866.5	1291	1291	685.1
Mass Flow [kg/h]	2.500e+004	7.580e+004	8.160e+004	1.919e+004
Std Ideal Liq Vol Flow [m3/h]	28.90	8.510	10.18	23.80
Molar Enthalpy [kcal/kgmole]	1196	997.0	-3752	1.047e+004
Molar Entropy [kJ/kgmole-C]	136.8	147.8	243.6	173.9
Heat Flow [kcal/h]	1.037e+006	1.288e+006	-4.846e+006	7.170e+006

Figure 8.10 Reactor 1 conditions



	Air to oxidizer	Ni to Oxidizer	12	11
Nitrogen	0.7900	**0.0000**	0.0000	0.9992
Hydrogen	0.0000	**0.0000**	0.0000	0.0000
CO2	0.0000	**0.0000**	0.0000	0.0000
CO	0.0000	**0.0000**	0.0000	0.0000
Oxygen	0.2100	**0.0000**	0.0000	0.0008
Methane	0.0000	**0.0000**	0.0000	0.0000
Nickel*	0.0000	**1.0000**	0.7190	0.0000
Nickel Oxide*	0.0000	**0.0000**	0.2810	0.0000
H2O	0.0000	**0.0000**	0.0000	0.0000

Figure 8.11 Reactor 1 worksheet



Name	**NiO to reducer**	**CH4 to Reducer**	**9**	**8**
Vapour	0.0000	1.0000	0.0000	1.0000
Temperature [C]	**800.0**	**216.8**	179.5	179.5
Pressure [bar]	29.67	29.99	29.67	29.67
Molar Flow [kgmole/h]	1291	779.2	1291	1142
Mass Flow [kg/h]	8.160e+004	1.250e+004	7.580e+004	1.831e+004
Std Ideal Liq Vol Flow [m3/h]	10.18	41.75	8.510	52.17
Molar Enthalpy [kcal/kgmole]	-9648	-1.610e+004	997.0	-2.302e+004
Molar Entropy [kJ/kgmole-C]	225.2	174.9	147.8	157.5
Heat Flow [kcal/h]	-1.246e+007	-1.254e+007	1.288e+006	-2.629e+007

Figure 8.12 Reactor 2 conditions

8.8 Cyclone Separator:

Cyclone separators are employed to separate solids and gases at the upstream of reactor. Cyclones are placed both after oxidizer and reducer. The worksheet shows the separation and efficiency of cyclones.

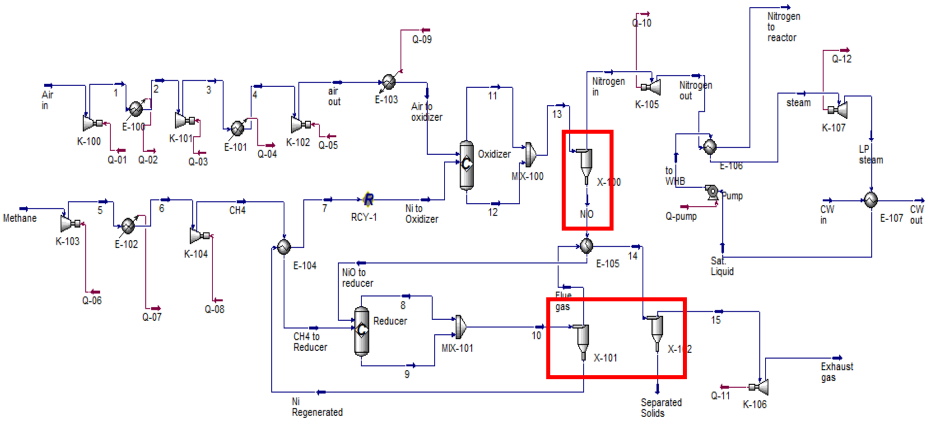
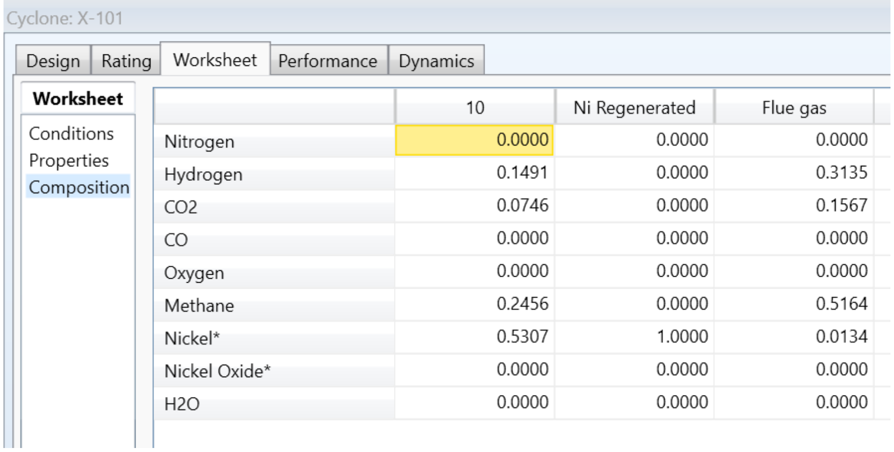
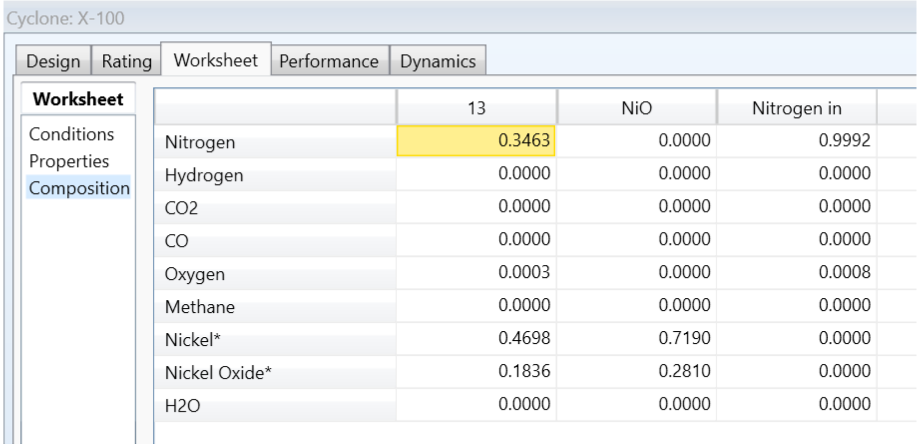


Figure 8.13 Cyclone separators



	10	Ni Regenerated	Flue gas
Nitrogen	0.0000	0.0000	0.0000
Hydrogen	0.1491	0.0000	0.3135
CO2	0.0746	0.0000	0.1567
CO	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000
Methane	0.2456	0.0000	0.5164
Nickel*	0.5307	1.0000	0.0134
Nickel Oxide*	0.0000	0.0000	0.0000
H2O	0.0000	0.0000	0.0000

Figure 8.14 Cyclone separator composition



	13	NiO	Nitrogen in
Nitrogen	0.3463	0.0000	0.9992
Hydrogen	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
CO	0.0000	0.0000	0.0000
Oxygen	0.0003	0.0000	0.0008
Methane	0.0000	0.0000	0.0000
Nickel*	0.4698	0.7190	0.0000
Nickel Oxide*	0.1836	0.2810	0.0000
H2O	0.0000	0.0000	0.0000

Figure 8.15 Cyclone separator composition

8.9 Gas Turbines:

Two gas turbines are employed downstream of cyclone separators, where pure gas at high temperature and pressure enter and expands, driving the turbine and generating energy which as a result is used in the process itself.

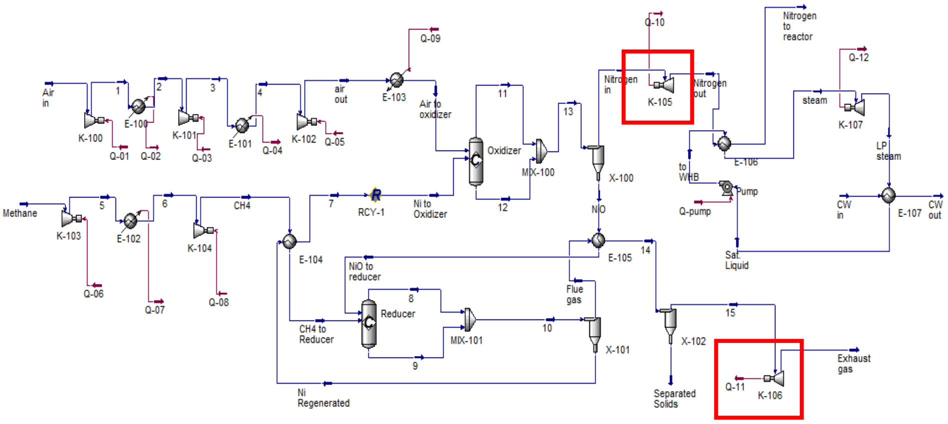
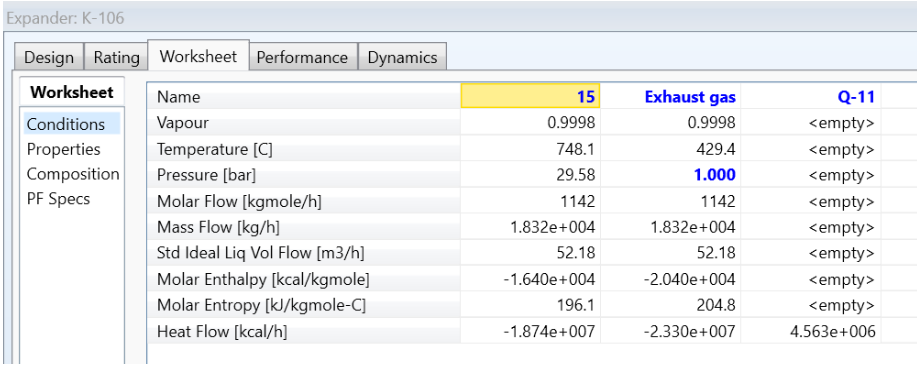
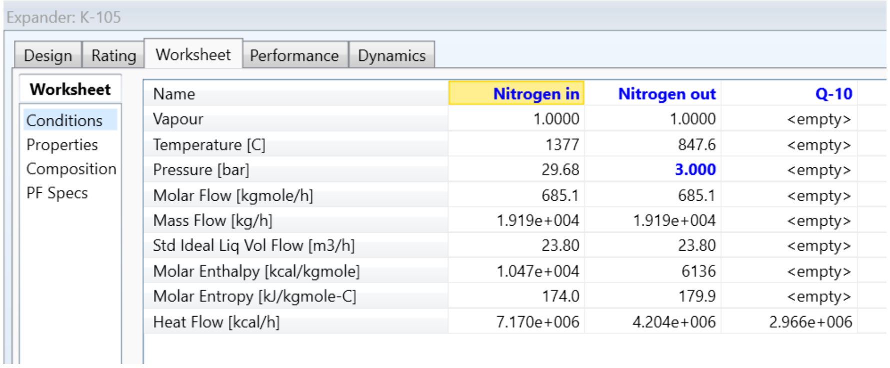


Figure 8.16 Gas turbine



Name	15	Exhaust gas	Q-11
Vapour	0.9998	0.9998	<empty>
Temperature [C]	748.1	429.4	<empty>
Pressure [bar]	29.58	1.000	<empty>
Molar Flow [kgmole/h]	1142	1142	<empty>
Mass Flow [kg/h]	1.832e+004	1.832e+004	<empty>
Std Ideal Liq Vol Flow [m3/h]	52.18	52.18	<empty>
Molar Enthalpy [kcal/kgmole]	-1.640e+004	-2.040e+004	<empty>
Molar Entropy [kJ/kgmole-C]	196.1	204.8	<empty>
Heat Flow [kcal/h]	-1.874e+007	-2.330e+007	4.563e+006

Figure 8.17 Gas turbine 1 worksheet



Name	Nitrogen in	Nitrogen out	Q-10
Vapour	1.0000	1.0000	<empty>
Temperature [C]	1377	847.6	<empty>
Pressure [bar]	29.68	3.000	<empty>
Molar Flow [kgmole/h]	685.1	685.1	<empty>
Mass Flow [kg/h]	1.919e+004	1.919e+004	<empty>
Std Ideal Liq Vol Flow [m3/h]	23.80	23.80	<empty>
Molar Enthalpy [kcal/kgmole]	1.047e+004	6136	<empty>
Molar Entropy [kJ/kgmole-C]	174.0	179.9	<empty>
Heat Flow [kcal/h]	7.170e+006	4.204e+006	2.966e+006

Figure 8.18 Gas turbine 2 worksheet

8.10 Steam engine:

It is employed for the purpose of heat recovery from the stream downstream of gas turbine. N2 gas at high temperature is use to generate steam. This HT and HP steam expands in steam turbine to generate energy, or this steam can be used in the form of steam as utility. Steam engine consist of turbine, pump, condenser, waste heat boiler (heat exchanger)

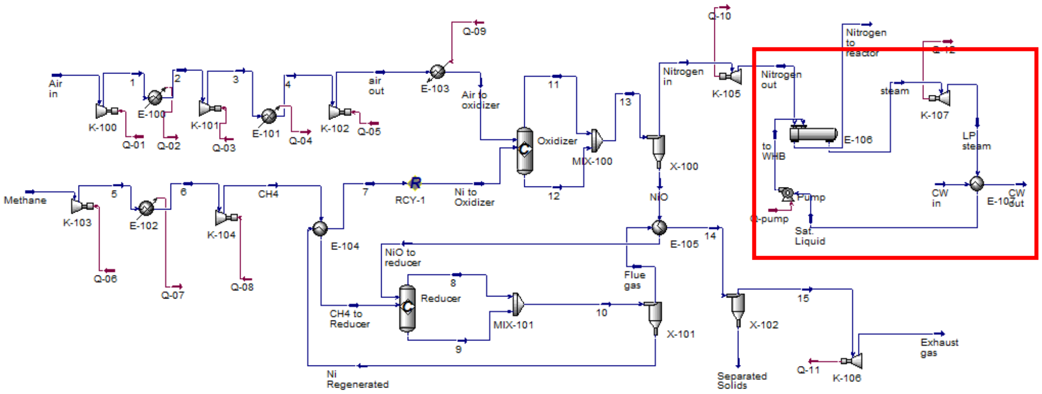
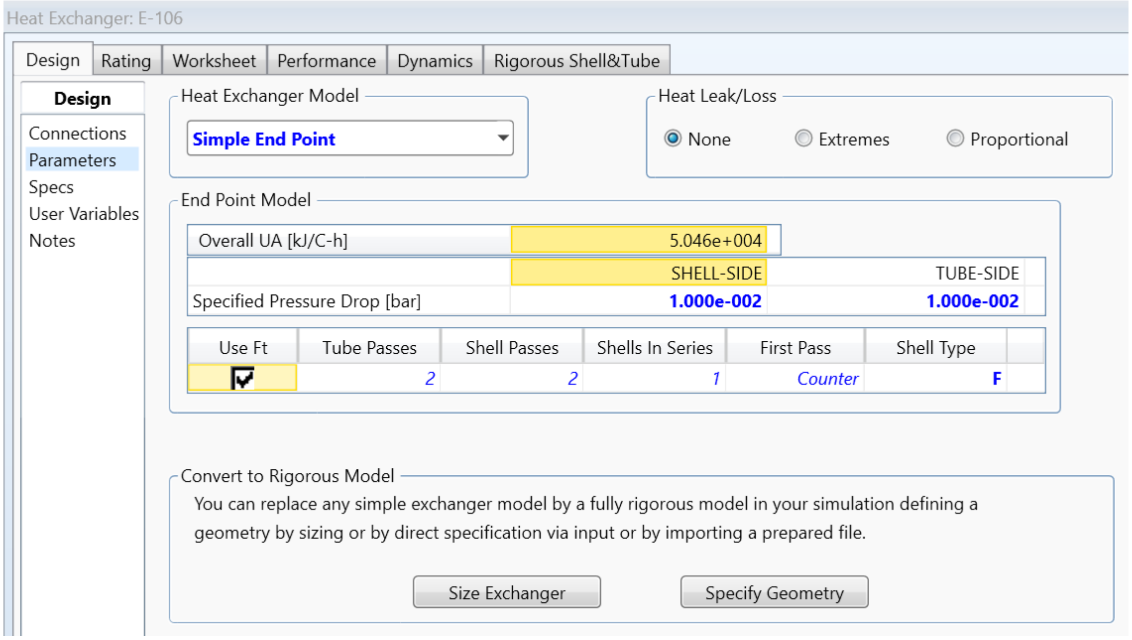


Figure 8.19 Steam engine

8.11 Waste Heat boiler:



Heat Exchanger Model: Simple End Point

Heat Leak/Loss: ● None ○ Extremes ○ Proportional

End Point Model

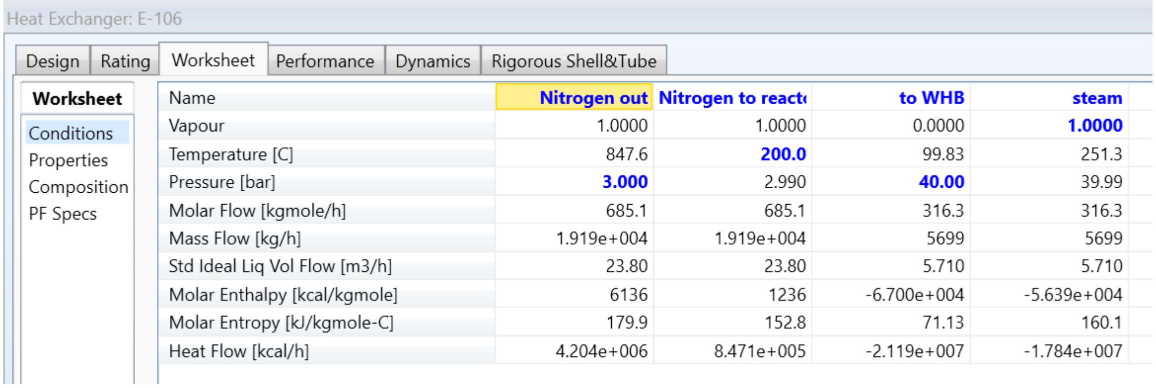
	SHELL-SIDE	TUBE-SIDE
Overall UA [kJ/C-h]	5.046e+004	
Specified Pressure Drop [bar]	1.000e-002	1.000e-002

Use Ft	Tube Passes	Shell Passes	Shells In Series	First Pass	Shell Type
☑	2	2	1	Counter	F

Convert to Rigorous Model

You can replace any simple exchanger model by a fully rigorous model in your simulation defining a geometry by sizing or by direct specification via input or by importing a prepared file.

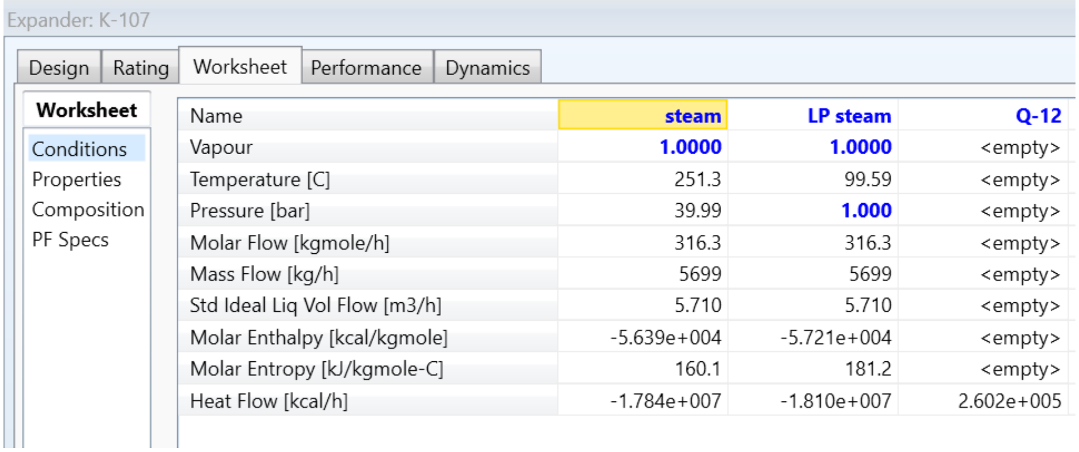
Figure 8.20 Waste heat boiler parameters



Name	Nitrogen out	Nitrogen to react	to WHB	steam
Vapour	1.0000	1.0000	0.0000	1.0000
Temperature [C]	847.6	200.0	99.83	251.3
Pressure [bar]	3.000	2.990	40.00	39.99
Molar Flow [kgmole/h]	685.1	685.1	316.3	316.3
Mass Flow [kg/h]	1.919e+004	1.919e+004	5699	5699
Std Ideal Liq Vol Flow [m3/h]	23.80	23.80	5.710	5.710
Molar Enthalpy [kcal/kgmole]	6136	1236	-6.700e+004	-5.639e+004
Molar Entropy [kJ/kgmole-C]	179.9	152.8	71.13	160.1
Heat Flow [kcal/h]	4.204e+006	8.471e+005	-2.119e+007	-1.784e+007

Figure 8.21 Waster heat boiler worksheet

8.12 Steam Turbine:

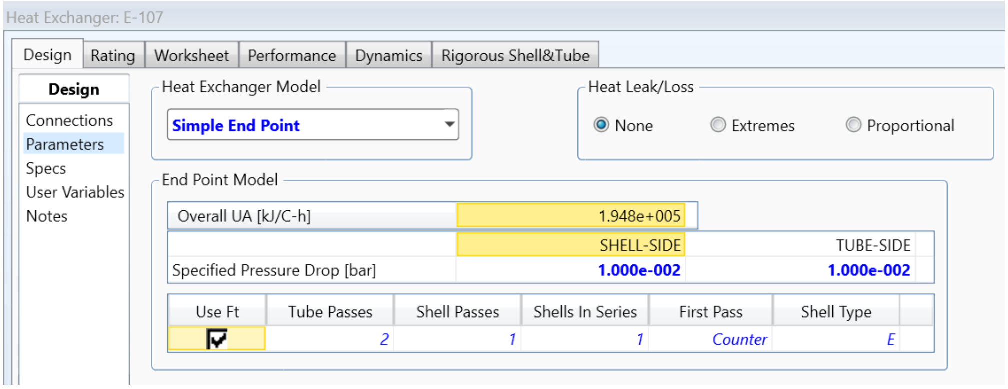


Name	steam	LP steam	Q-12
Vapour	1.0000	1.0000	<empty>
Temperature [C]	251.3	99.59	<empty>
Pressure [bar]	39.99	1.000	<empty>
Molar Flow [kgmole/h]	316.3	316.3	<empty>
Mass Flow [kg/h]	5699	5699	<empty>
Std Ideal Liq Vol Flow [m3/h]	5.710	5.710	<empty>
Molar Enthalpy [kcal/kgmole]	-5.639e+004	-5.721e+004	<empty>
Molar Entropy [kJ/kgmole-C]	160.1	181.2	<empty>
Heat Flow [kcal/h]	-1.784e+007	-1.810e+007	2.602e+005

Figure 8.22 Steam turbine worksheet

8.13 Condenser:

To condense steam to saturated liquid. At 1 bar, the saturated liquid temperature is 100C.



Heat Exchanger Model: Simple End Point

Heat Leak/Loss: ● None ○ Extremes ○ Proportional

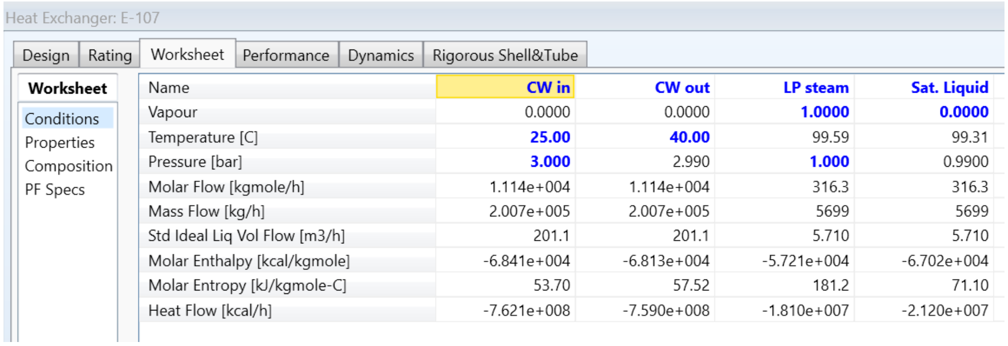
End Point Model

Overall UA [kJ/C-h]	1.948e+005

	SHELL-SIDE	TUBE-SIDE
Specified Pressure Drop [bar]	1.000e-002	1.000e-002

Use Ft	Tube Passes	Shell Passes	Shells In Series	First Pass	Shell Type
☑	2	1	1	Counter	E

Figure 8.23 Condenser parameters

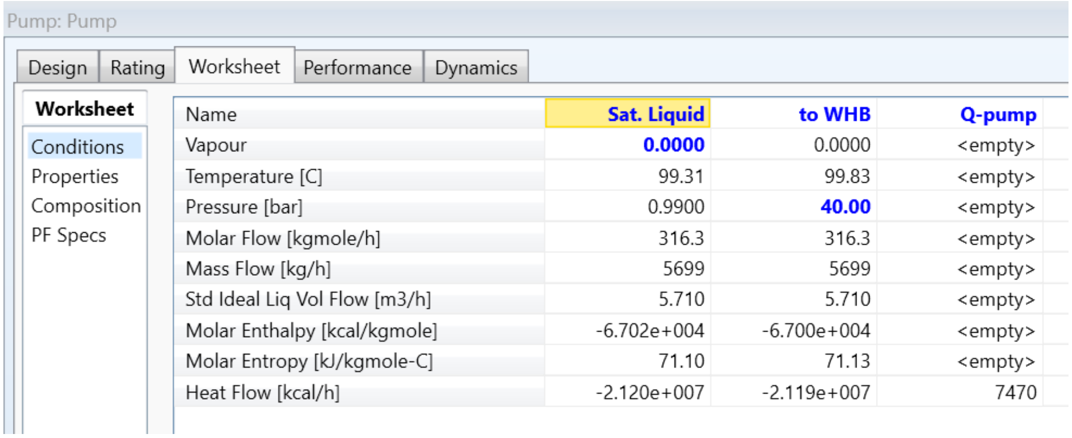


Name	CW in	CW out	LP steam	Sat. Liquid
Vapour	0.0000	0.0000	1.0000	0.0000
Temperature [C]	25.00	40.00	99.59	99.31
Pressure [bar]	3.000	2.990	1.000	0.9900
Molar Flow [kgmole/h]	1.114e+004	1.114e+004	316.3	316.3
Mass Flow [kg/h]	2.007e+005	2.007e+005	5699	5699
Std Ideal Liq Vol Flow [m3/h]	201.1	201.1	5.710	5.710
Molar Enthalpy [kcal/kgmole]	-6.841e+004	-6.813e+004	-5.721e+004	-6.702e+004
Molar Entropy [kJ/kgmole-C]	53.70	57.52	181.2	71.10
Heat Flow [kcal/h]	-7.621e+008	-7.590e+008	-1.810e+007	-2.120e+007

Figure 8.24 Condenser worksheet

8.14 Pump:

To increase the pressure of saturated liquid from 1 to 40 bar.

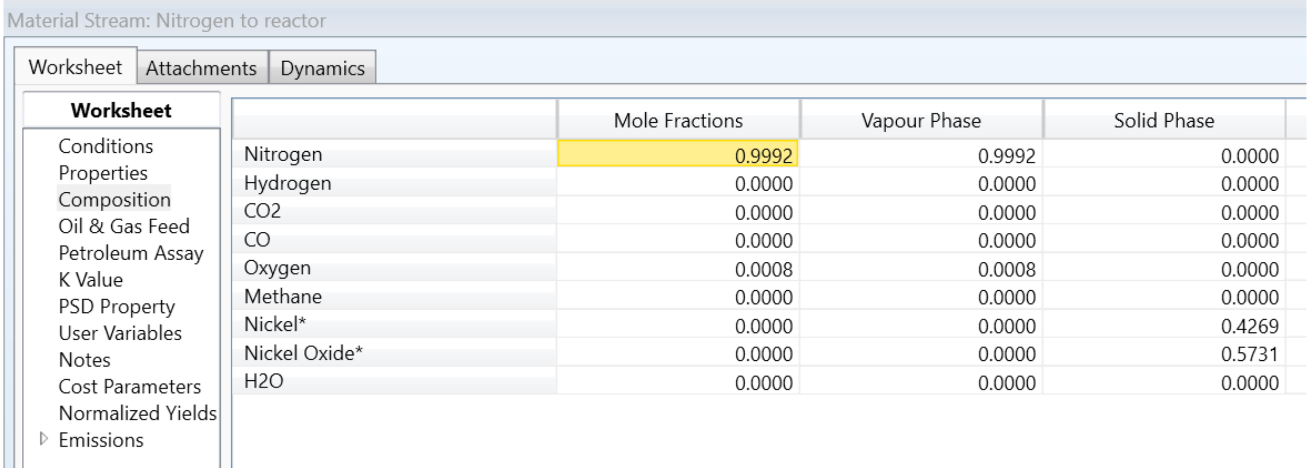


Name	Sat. Liquid	to WHB	Q-pump
Vapour	0.0000	0.0000	<empty>
Temperature [C]	99.31	99.83	<empty>
Pressure [bar]	0.9900	40.00	<empty>
Molar Flow [kgmole/h]	316.3	316.3	<empty>
Mass Flow [kg/h]	5699	5699	<empty>
Std Ideal Liq Vol Flow [m3/h]	5.710	5.710	<empty>
Molar Enthalpy [kcal/kgmole]	-6.702e+004	-6.700e+004	<empty>
Molar Entropy [kJ/kgmole-C]	71.10	71.13	<empty>
Heat Flow [kcal/h]	-2.120e+007	-2.119e+007	7470

Figure 8.25 Pump worksheet

8.15 Product Stream:

Nitrogen gas with following specifications is obtained, that can be seen from the composition sheet. Simulation validates the manual calculations, as nitrogen 19100 kg/hr is produced with purity of 99.4%.



	Mole Fractions	Vapour Phase	Solid Phase
Nitrogen	0.9992	0.9992	0.0000
Hydrogen	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
CO	0.0000	0.0000	0.0000
Oxygen	0.0008	0.0008	0.0000
Methane	0.0000	0.0000	0.0000
Nickel*	0.0000	0.0000	0.4269
Nickel Oxide*	0.0000	0.0000	0.5731
H2O	0.0000	0.0000	0.0000

Figure 8.26 Product stream worksheet

CHAPTER 9

ECONOMIC ANALYSIS

9.1 Cost Estimations Economic Analysis

The economic viability of a project is a crucial determinant of its feasibility. Conducting a comprehensive economic analysis is essential to evaluate the financial aspects of the project and its components. As the primary objective of any project is to generate revenue and engage in business activities, cost plays a pivotal role in making decisions regarding equipment installations. Efficient project management heavily relies on effectively managing costs, as they significantly impact the project's outcomes. It is often necessary to balance time and quality considerations with the cost factor to achieve the desired results within budgetary constraints. For this project, we have adopted the Coulson and Richardson method for conducting a thorough economic analysis. This method provides a structured framework to assess the economic viability and make informed decisions regarding the project's financial aspects. Following are some of the costs calculated.

1. **Purchased cost of equipment (PCE):** This cost is of solely equipments purchased, no operation or installation cost is included in this. This cost is calculated by the graphs and formulas (correlations) given by Coulson.

2. **Physical Plant Cost (PPC):** This is the PCE in addition with the cost of building, labors, utilities. In conclusion, the cost required for the one-time installation of the equipment.

3. **Fixed Capital (FC):** This is the PPC in addition to design and engineering, contractors fee etc. In conclusion, this is the total investment required before starting the process. This does not include any operating cost.

4. **Annual Operating Cost:** This is the sum of fixed operating cost and variable operating cost. In conclusion this is the cost used to run the plant daily, includes utilities, raw material, labor, plant supervision, engineer’s fee, plant overheads, taxes, insurance, R&D.

5. **Total Revenue:** Amount the company receives by selling the end product to consumers, this also includes the amount invested to generate that revenue (operating cost).

6. **Profit:** Total revenue minus the operating cost of the equipment. This is the profit generated by selling the end product.

7. **Payback period:** The payback period demonstrates when does the initial investment is returned. It is the ratio of total initial investment (Fixed capital) and the profit generated. For an ideal business the payback is usually 2 -4 years. The payback period shows the economic feasibility and profitability of the business.

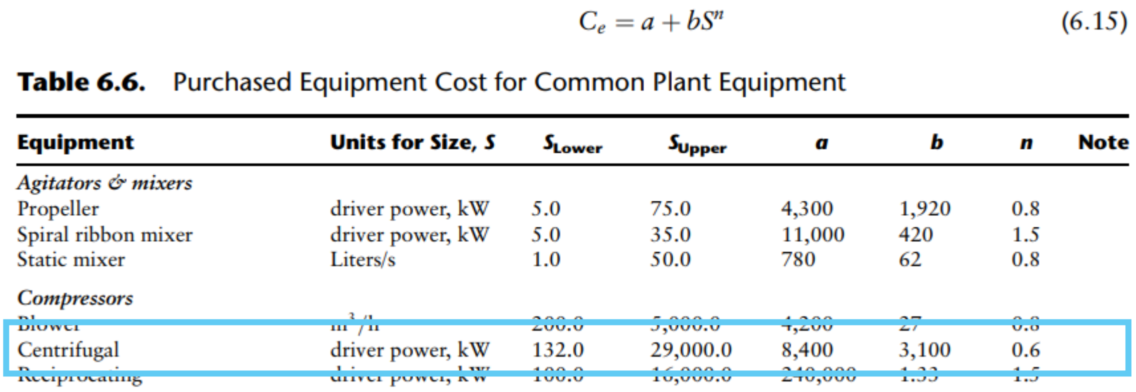
9.2 Purchase Cost of Equipment:

9.2.1 Multistage Compressors:

Formula: $Ce = a + bS^n$

Values for a, b, n given in the following table:

Table 9.1 PCE for Common plant equipment



$$C_e = a + bS^n \qquad (6.15)$$

Table 6.6. Purchased Equipment Cost for Common Plant Equipment

Equipment	Units for Size, S	S_{Lower}	S_{Upper}	a	b	n	Note
Agitators & mixers							
Propeller	driver power, kW	5.0	75.0	4,300	1,920	0.8	
Spiral ribbon mixer	driver power, kW	5.0	35.0	11,000	420	1.5	
Static mixer	Liters/s	1.0	50.0	780	62	0.8	
Compressors							
Blower	m^3/h	200.0	5,000.0	4,200	27	0.8	
Centrifugal	driver power, kW	132.0	29,000.0	8,400	3,100	0.6	
Reciprocating	driver power, kW	100.0	16,000.0	240,000	1.33	1.5	

Air compressor Duty (S) = 3324 kW

Ce = 410522 $

Fuel Compressor Duty (S) = Duty = 2000 kW

Ce = 304869 $

9.2.2 Oxidizer and Reducer:

Reactor consists of:

1. A vessel
2. Oxygen carrier as Ni particles
3. A perforated plate as air distributor

Vessel height = 8.4m

Vessel diameter = 2.8 m

Perforated Plate diameter = 2.8m

Material = C.S

Pressure = 30 bar

Formula: $Ce = CS^n$

Vessel cost = 49000$

Plate cost = 1000$

Ni cost per kg = 19$

Ni cost = 38000$

Total reactor cost = 88000$

Cost for 2 reactors = 176000$

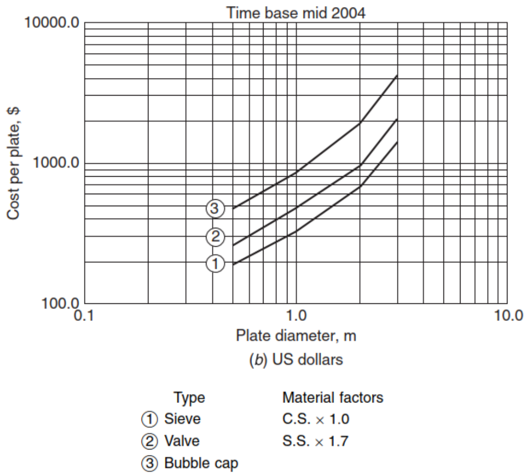


Figure 9.1 Plate cost graph

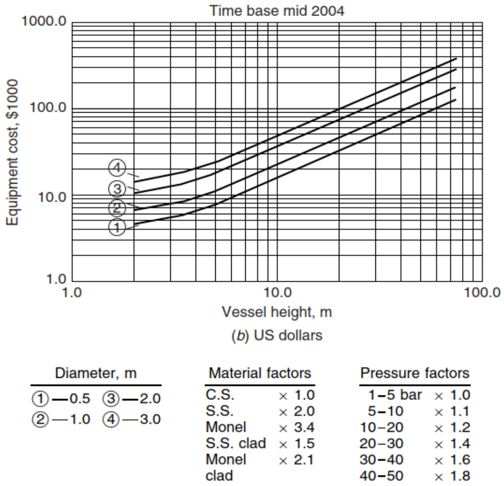


Figure 9.2 Vessel cost graph

9.2.3 Cyclone Separator:

Formula: Ce = CS^n

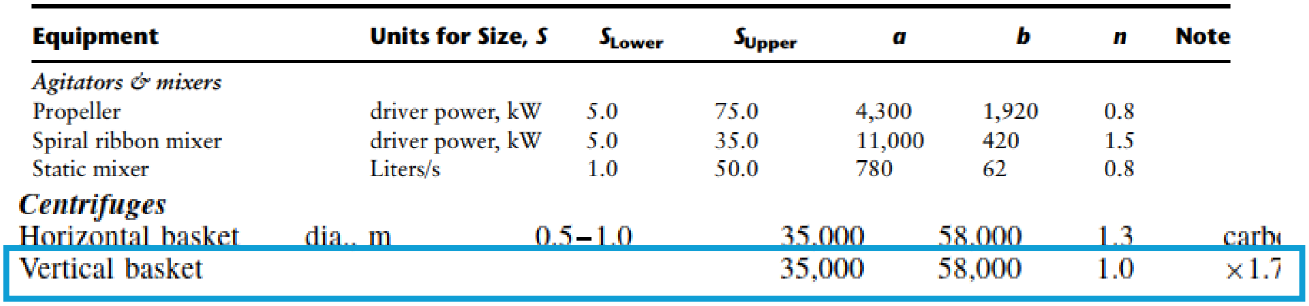
Diameter 9S) = 0.46 m

Formula: Ce = $a + bS^n$

Ce = 61680 $

Cost for 5 cyclone separators= 308400 $

Table 9.2 PCE for Common plant equipment



Equipment	**Units for Size, *S***	***S***					

9.2.4 Pump:

Formula: Ce = CS^n

Table 9.3 PCE for Common plant equipment

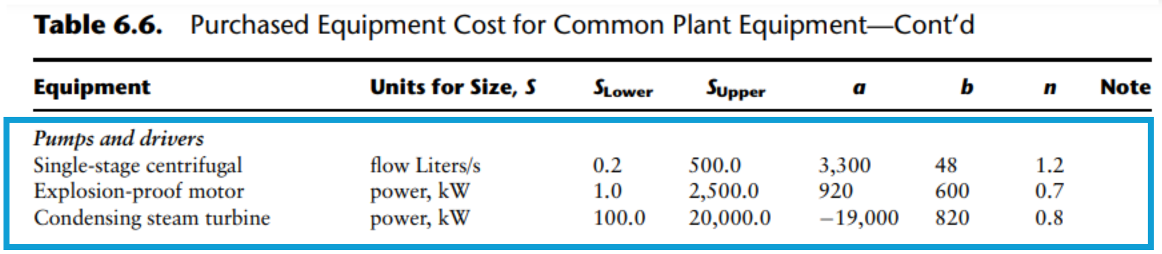


Table 6.6. Purchased Equipment Cost for Common Plant Equipment—Cont'd

Equipment	Units for Size, *S*	S_{Lower}	S_{Upper}	*a*	*b*	*n*	Note
Pumps and drivers							
Single-stage centrifugal	flow Liters/s	0.2	500.0	3,300	48	1.2	
Explosion-proof motor	power, kW	1.0	2,500.0	920	600	0.7	
Condensing steam turbine	power, kW	100.0	20,000.0	−19,000	820	0.8	

Pump Duty (S) = 8.6 kW

Ce = 3934$

9.2.5 Gas Turbines:

Formula: Ce = CS^n

Gas Turbine-01 Duty = 3448 kW

Ce = 176159$

Gas turbine – 02 Duty = 5303 kW

Table 9.4 PCE for miscellaneous equipment

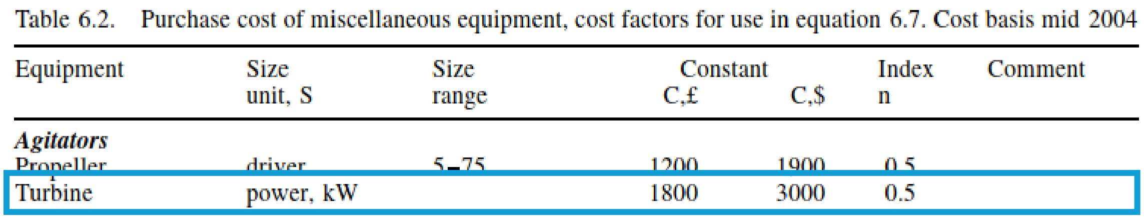


Table 6.2. Purchase cost of miscellaneous equipment, cost factors for use in equation 6.7. Cost basis mid 2004

Equipment	Size unit, S	Size range	Constant C,£	Constant C,$	Index n	Comment
Agitators						
Propeller	driver	5–75	1200	1900	0.5	
Turbine	power, kW		1800	3000	0.5	

9.2.6 Steam Turbine:

Formula: $Ce = CS^n$

Duty = 302 kW

Table 9.5 PCE for miscellaneous equipment

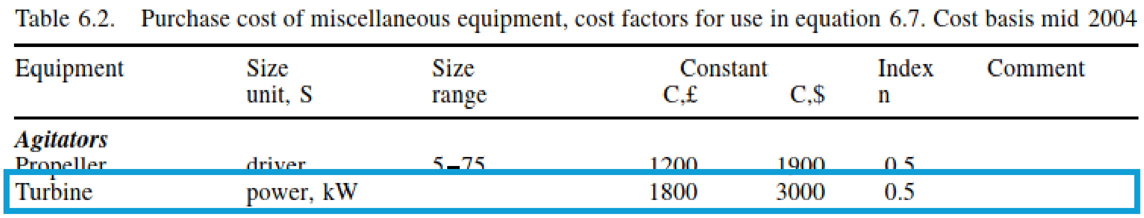


Table 6.2. Purchase cost of miscellaneous equipment, cost factors for use in equation 6.7. Cost basis mid 2004

Equipment	Size unit, S	Size range	Constant C,£	C,$	Index n	Comment
Agitators						
Propeller	driver	5–75	1200	1900	0.5	
Turbine	power, kW		1800	3000	0.5	

9.2.7 Condenser (Shell & Tube type):

Heat Transfer area = 142 m^2

Floating head type

Material = C.S

Pressure = 1-2 bar

Fluid = water (non- corrosive)

Formula = cost from graph x Type factor x Pressure factor

Cost (from graph) = 35,000$

9.2.8 Waste Heat Boiler (Shell & Tube type):

Heat Transfer area = 60 m^2

Floating head type

Material = C.S

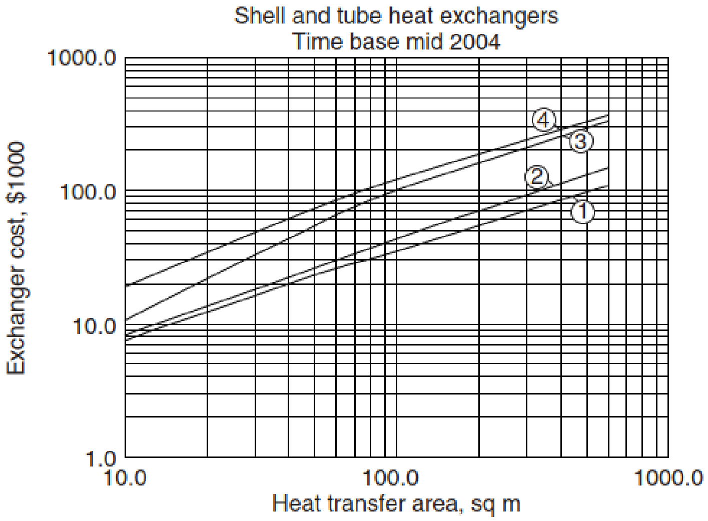
Pressure = 40 bar

Fluid = water (non- corrosive)

Pressure factor = 1.3

Formula = cost from graph x Type factor x Pressure factor

Cost (from graph) = 39,000$



(b) US dollars

Materials	
Shell	Tubes
① Carbon steel	Carbon steel
② C.S.	Brass
③ C.S.	Stainless steel
④ S.S.	S.S.

Pressure factors	
1–10 bar	× 1.0
10–20	× 1.1
20–30	× 1.25
30–50	× 1.3
50–70	× 1.5

Type factors	
Floating head	× 1.0
Fixed tube sheet	× 0.8
U tube	× 0.85
Kettle	× 1.3

Figure 6.3*a*, *b*. Shell and tube heat exchangers. Time base mid-2004
Purchased cost = (bare cost from figure) × Type factor × Pressure factor

Figure 9.3 Cost of Heat exchanger graph

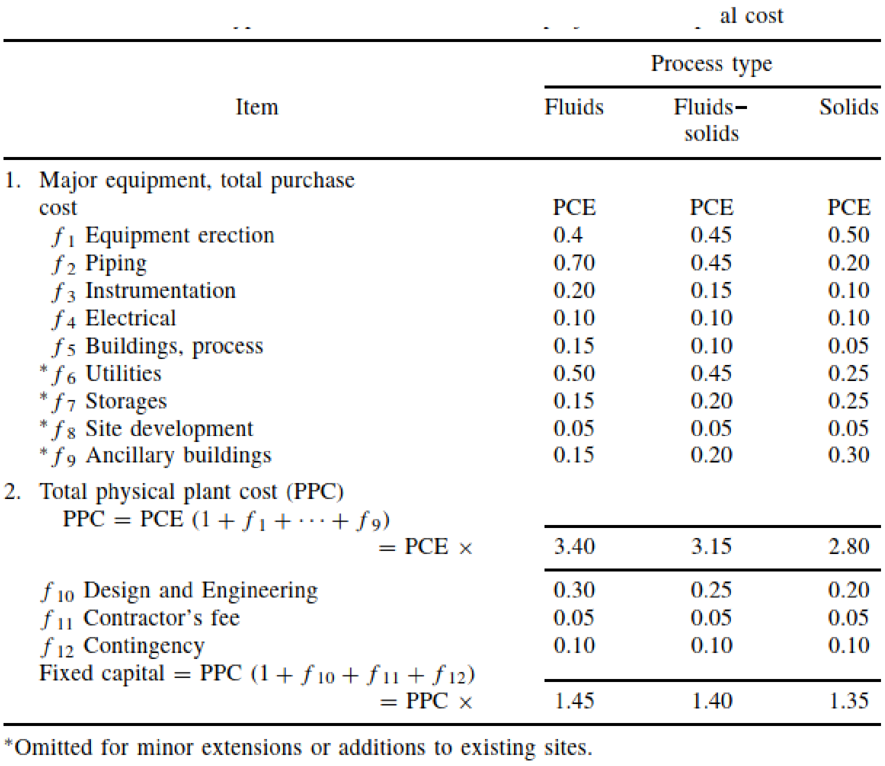
Table 9.6 Purchase cost of equipment

Equipment	Cost ($)
Multistage compressor -01	410522
Multistage compressor -02	304869
Reactors	176000
Cyclone Separator	308400
Gas Turbine - 01	218465
Gas Turbine - 02	176159
Steam Turbine	60034
Pump	3934
WHB	39000
Condenser	35000
Purchase Cost of Equipment	1697383

Total PCE in 2004 = $1697383

Total PCE in 2024 = $3055289.6

Table 9.7 Factors for estimation of Fixed capital cost



al cost

Item	Process type		
	Fluids	Fluids–solids	Solids
1. Major equipment, total purchase cost	PCE	PCE	PCE
f_1 Equipment erection	0.4	0.45	0.50
f_2 Piping	0.70	0.45	0.20
f_3 Instrumentation	0.20	0.15	0.10
f_4 Electrical	0.10	0.10	0.10
f_5 Buildings, process	0.15	0.10	0.05
* f_6 Utilities	0.50	0.45	0.25
* f_7 Storages	0.15	0.20	0.25
* f_8 Site development	0.05	0.05	0.05
* f_9 Ancillary buildings	0.15	0.20	0.30
2. Total physical plant cost (PPC)			
$\text{PPC} = \text{PCE}\ (1 + f_1 + \cdots + f_9)$			
$= \text{PCE} \times$	3.40	3.15	2.80
f_{10} Design and Engineering	0.30	0.25	0.20
f_{11} Contractor's fee	0.05	0.05	0.05
f_{12} Contingency	0.10	0.10	0.10
$\text{Fixed capital} = \text{PPC}\ (1 + f_{10} + f_{11} + f_{12})$			
$= \text{PPC} \times$	1.45	1.40	1.35

*Omitted for minor extensions or additions to existing sites.

PPC = PCE x 3.15 (For fluids, solids)

PPC = 3055289.6 x 3.15 = 9624162.178$

PPC= 9624162.178$

Fixed Capital = PPC x 1.40

Fixed capital = 13473827$

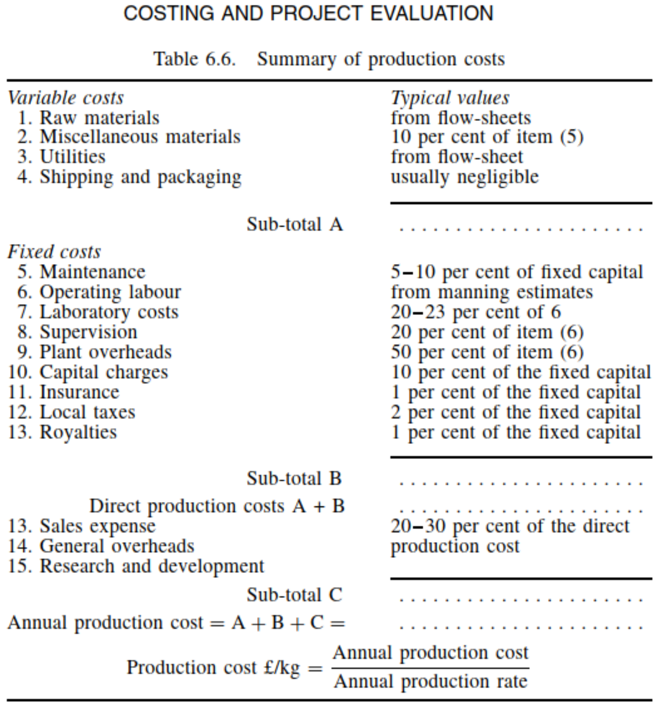
Working capital (WC) = 5% of FC

Working capital = 673691$

Total Investment = FC + WC

Total investment = 14147518$

Table 9.8 Summary of production costs



COSTING AND PROJECT EVALUATION

Table 6.6. Summary of production costs

Variable costs	*Typical values*
1. Raw materials	from flow-sheets
2. Miscellaneous materials	10 per cent of item (5)
3. Utilities	from flow-sheet
4. Shipping and packaging	usually negligible
Sub-total A	. . . .
Fixed costs	
5. Maintenance	5–10 per cent of fixed capital
6. Operating labour	from manning estimates
7. Laboratory costs	20–23 per cent of 6
8. Supervision	20 per cent of item (6)
9. Plant overheads	50 per cent of item (6)
10. Capital charges	10 per cent of the fixed capital
11. Insurance	1 per cent of the fixed capital
12. Local taxes	2 per cent of the fixed capital
13. Royalties	1 per cent of the fixed capital
Sub-total B	. . . .
Direct production costs A + B	. . . .
13. Sales expense 14. General overheads 15. Research and development	20–30 per cent of the direct production cost
Sub-total C	. . . .
Annual production cost = A + B + C =	. . . .

$$\text{Production cost £/kg} = \frac{\text{Annual production cost}}{\text{Annual production rate}}$$

Table 9.9 Costing summary

Operating time of plant	347 days
Total Investment	15M
Annual operating cost	11.3M
Revenue	16.7M
Profit	5.4M
Payback period	2.7 years

CHAPTER 10

INSTRUMENTATION

10.1 Cascade control loop

A cascade control loop, also known as a nested control loop, is a control system configuration where two or more control loops are interconnected to improve the overall control performance. In a cascade control loop, there are typically two levels of control: the primary or outer loop and the secondary or inner loop. Temperature controller is the primary controller and flowrate controller is the secondary controller. Required temperature is the setpoint and the manipulated variable is the valve adjustment. Main reason of using cascade loop is to maintain the temperature at desired value or sets point. The flowrate can be adjusted to maintain the temperature at required level.

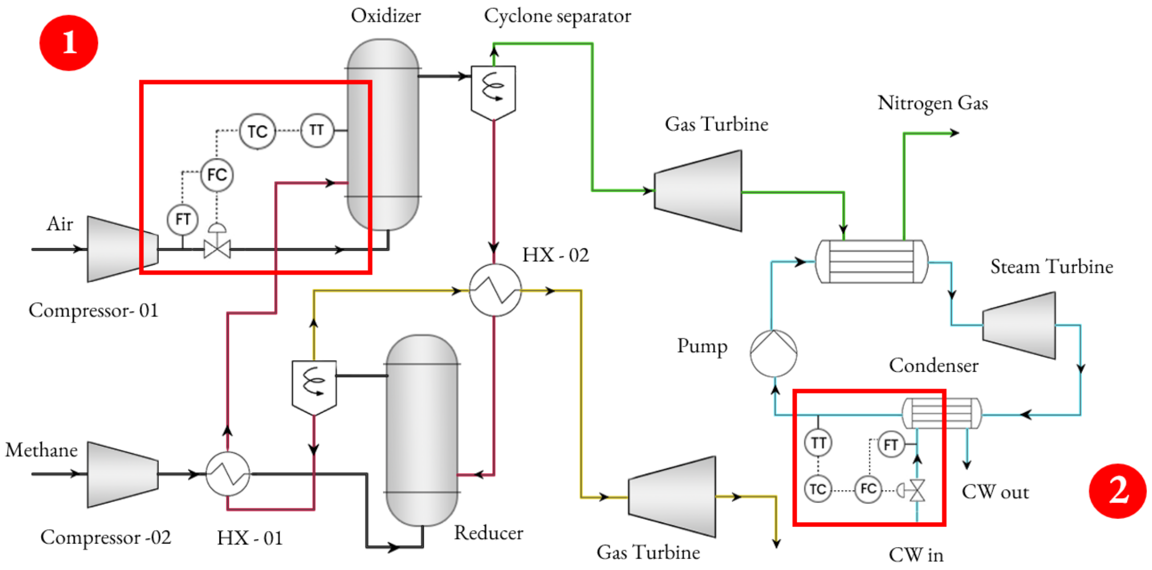


Figure 10.1 Cascade control loop

10.1.1 Cascade control loop on condenser:

The cascade control loop involves two variables, namely temperature and flow rate. In this setup, temperature acts as the primary control loop, while flow rate serves as the secondary control loop. The objective is to maintain the temperature of the stream after the condenser at 100°C at 1 bar pressure, a task handled by the temperature control mechanism. This control is achieved by regulating the flow rate of the cooling water.

Maintaining the temperature is crucial downstream of the condenser because it ensures that the saturated liquid entering the pump is at the desired state. Any presence of vapor in the stream can adversely affect the pump's lifespan and performance. To address this issue, a cascade control system is implemented. It continuously adjusts the temperature by modulating the flow rate of the cooling water whenever the temperature deviates from the setpoint of 100°C.

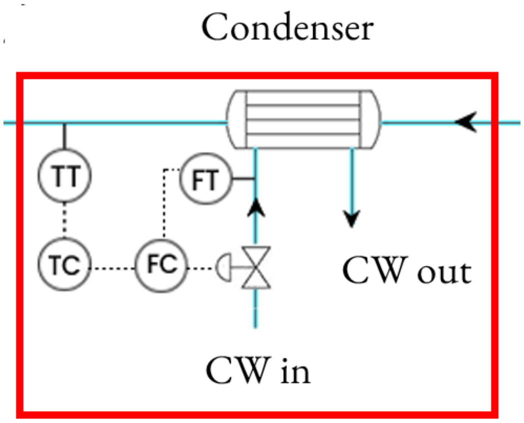


Figure 10.2 Control loop on condenser

10.1.2 Cascade control loop on oxidizer:

In this setup, temperature acts as the primary control loop, while flow rate serves as the secondary control loop. The objective is to maintain the temperature of reactor around 1200°C this is because Nickel inside the reactor melts at 1400°C which will cause the failure of the process. This temperature of the reactor is controlled by the inlet flow rate of air, as the reaction is exothermic, more heat is liberated and temperature is increased at higher air flow rate.

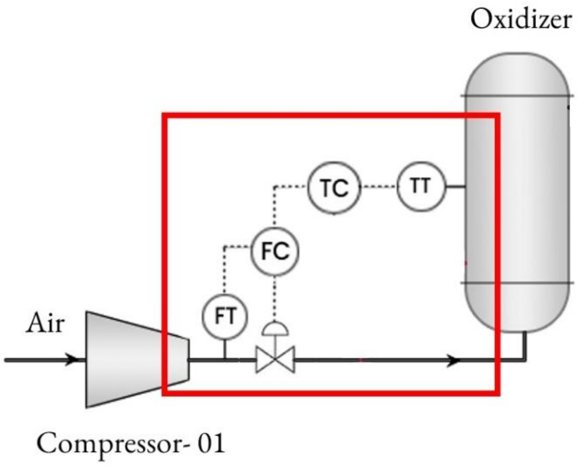


Figure 10.3 Control loop on oxidizer

CHAPTER 11

HAZOP ANALYSIS

11.1 Introduction:

Hazard and operability analysis, or HAZOP, is a thorough and systematic technique to perform risk assessment in a structured manner and identify potential hazards that could lead to catastrophic incidents. It is essential to maintain plant's safety and efficiency while putting employee's well-being first. HAZOP contributes to predictable production of requires products by implementing a variety of procedures, which in turn increases profitability [1].

11.2 Hazard identification:

The following are included in Hazard identification:

- **Process Hazards Checklists**

  Process hazards checklist is the list of items and possible problems in the process that must be checked in performing hazard assessments. This checklist's main objective is to find potential health and safety risks by looking at workplace policies or procedures.

- **Hazards Surveys**

  An inspection and report on buildings and structures for materials that could be detrimental to the health of workers, building occupants, or the environment make up a hazardous materials survey.

- **Hazards and Operability Studies**

  Various events are suggested for a specific piece of equipment with the participants determining whether and how the event could occur and whether the event creates any form of risk. It is important for consistent production of desired product which will increase the profitability of the process.

- **Safety review**

  A safety review is a comprehensive inspection of a jobsite with the goal of identifying risk and safety concerns. It also evaluates the productivity of the company's safety efforts and programs [2].

11.3 Health and Safety Communication:

- All employees receive periodic training on risk prevention and occupational health and safety.
- Installation of Hazard safety signs in accordance with international and national standards.
- Correct labeling and tagging of all equipment.
- Demarcation of different areas of the plant and walkways.
- Availability of instruction manuals for different equipment.
- Establishment of access point to material safety data sheet.

11.4 HAZOP on Heat exchanger:

Table 11.1 HAZOP on Heat exchanger

Parameter	Guide word	Deviation	Causes	Consequences	Action
Flow	**Less**	Less flow of gas in Heat exchanger	Line blockage Valve malfunctioning Complete leakage.	No heat transfers. Higher temperature of product.	Installation of Flow alarms Temperature sensors at outlet. Implementation of control for

			Line leakage	Equipment may overheat	flow rates of streams
	More	More than optimal flow to Heat Exchanger	Failure of inlet valve to close	Less than required temperature of existing stream achieved. Incomplete Heat exchanger	Installation of temperature alarms. Installation of flow meters. High pressure alarms for safety consideration
	Reverse	Black flow of gas due to high back pressure	Blockage at inlet or outlet of shell or tube. Valve at outlet fails to open	No heat exchange	Installation of automatic sensors and control devices. Installation of Non-Return Valves
Temperature	**High**	High Temp	High heating supply Temp.	Desired outlet temperature not achieved	Installation of flow and temperature alarms

			Less flow of coolant		
	Low	Low Temp	Low heating supply Temp More flow of coolant	Improper heat exchange. Desired outlet temperature not achieved	Installation of controllers
Pressure	**High**	High Pressure	Product line blockage. High Temperature leading to high pressure.	Improper heat exchange. Heat exchanger burst at high pressure	Installation of High-pressure alarms Installation of PSV’s
	Low	Low Pressure	Leakage in shell or tube	Desired exchange of heat not achieved	Check for leakages. Installation of low-pressure sensors. Proper maintenance

11.5 HAZOP on Pump:

Table 11.2 HAZOP on Pump

Parameter	Guide word	Deviation	Causes	Consequences	Action
Flow	**No**	No flow at the exit of pump	Blocked pipelines. Pump malfunctioning. Outlet valve fails to open	Pump overheating. Line overpressure	Proper monitoring of pumps. Installation of alarms on valve
	More	More flow than required	Too High shaft power. Valve opening failure. Blockade in valve outlet	Damage to pump due to cavitation. Pump overheating	Decrease the speed of shaft rotation. Check operating procedures
	Less	Less flow than required	Low rotational speed of shaft. Improper suction at inlet.	Pump overheating Pressure buildup	Increase speed of shaft rotation. Installation of controllers to

			Partial opening of downstream valve		operate valve according to flow
Pressure	**No**	No pressure	Pump failure. Power outage. Faulty pressure sensor. Shaft malfunctioning	Cavitation. Production stopped.	Proper maintenance. Check liquid type. Make sure NPSHA > NPSHR
	More	More pressure inside pump	Faulty pressure sensor	Bursting. Deterioration of bearings. Increased leakage. Production is stopped	Installation of high-pressure alarms
	Low	Low pressure inside pump	Pump malfunctioning. Power outage.	Cavitation. Deterioration of bearings	Proper maintenance. Check filters.

			Faulty pressure sensor Air leakage in suction line. Suction valve closed.		Make sure NPSHA > NPSHR

11.4 HAZOP on Fluidized Bed Reactor:

Table 11.3 HAZOP on Fluidized bed reactor

Parameter	Guide word	Deviation	Causes	Consequences	Action
Flow	**No**	Now flow of reactant	Feed line valve is closed. Feed line blockage. Pipe rupture. Equipment failure	No reaction takes place. Excess reactant in reactor	Regular inspection of pipelines. Proper maintenance of valves and pipelines
	Less	Less flow of reactant	Valve is partially closed.	Loss of reactant. Unreacted reactant.	Installation of flow control valves.

			Leakage in pipe	Product specifications not met	Regular inspection of pipelines. Recycling of unconverted reactant. Repairing of damaged pipelines
	More	More flow of reactant	Excessive pump speed. Malfunctioning of flow control valve	Pressure increase. Temperature fluctuation which may change reaction kinetics	Regular inspections of pump motors. Install high level alarms
	As well as	Other material enters	Contamination of raw material	Incomplete reaction. Desired product not achieved	Shut down of equipment. Check composition of feed in storage and reactant entering reactor

Temperature	**High**	High Temp	Desired operating temperature not achieved	Incomplete combustion or Reaction	Check Heating system
	Low	Low Temp	Feed line is loose	Incomplete combustion or reaction	Repair pipeline
Pressure	**High**	High Pressure	Failure of valve. Downstream of equipment. Fouling	Bursting of reactor due to pressure buildup	Emergency shutdown. Installation of relief valve. Regular inspection of equipment
	Low	Low Pressure	Opening of pressure control valve	Required conversion not achieved	Install pressure control loop

CONCLUSION

In summary, the project involves producing nitrogen gas from air at a rate of 19100 kg/hr, achieving a purity of 99.4%. Through design calculations and economic analysis, it has been determined that the project is feasible and capable of generating nitrogen gas. The proposed design, with a payback duration of 2.7 years, demonstrates cost-effectiveness and profitability, making it a valuable addition to the plant and beneficial for the economy. The process, named for its combustion-based method, regenerates energy through exothermic reactions, reducing overall energy consumption and the need for additional utilities such as electricity or steam.

Furthermore, the process aligns with the United Nations' 8th and 9th Sustainable Development Goals:

1. Decent work and economic growth

2. Industry innovation and infrastructure development

Comparison of nitrogen production technologies; PSA, Liquefaction, Combustion-based:

1. Purity: While PSA and liquefaction technologies achieve a higher purity of 99.99%, combustion-based technology produces nitrogen gas with a purity of 99.4%.

2. Energy Consumption: Combustion-based technology is more energy efficient and generates energy as a byproduct of the process. In contrast, PSA and liquefaction technologies require substantial energy inputs to achieve high pressure (in PSA) and low temperatures (in liquefaction).

3. Process Complexity: PSA is simpler to operate compared to combustion-based and liquefaction technologies. This results in increased maintenance requirements, labor, and control measures for the plant.

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