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Production of 6 MMSCFD of Synthetic Natural Gas via Thermochemical Conversion of Solid Waste

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Production of 3.6 million ft3 / day of Synthetic Natural Gas through Thermochemical Conversion of Solid Waste

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This report is submitted to the Department of Chemical Engineering, Wah Engineering College, University of Wah for the partial fulfilments of the requirement for the

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Department of Chemical Engineering,
Wah Engineering College,
University of Wah
Wah Cantt.

Dedication

“Educating the mind without educating the heart is no education at all.”

-Aristotle

We devote our humble effort to our lovely,

Parents

Whose devotion, support, encouragement, and prayers of day and night enable us to achieve such success and honor.

Along with anyone who is diligent and respected,

Teachers

Acknowledgement

All praise be to **Allah**, the lord of the worlds, who has conferred on us such an opportunity to go through a splendid journey by bestowment of his kindness and mercy in completing this project.

The trail to this work was quite protracted and not smooth, but finally the end was reached via efforts of many sleepless nights and redressing of mistakes. This would probably not have happened had our guides not been there on the way. For this we'd like to thank our parents for their unwavering support and unconditional love; they kept us moving and this project would not have been possible without them.

We would like to express our heartfelt gratitude to our supervisors, **Dr. Saleem Iqbal** and **Engr. Aasia Farrukh,** who have provided us with invaluable direction, support, and inspiration for us to finish this thesis successfully. Our gratitude to the entire **Chemical Engineering Faculty**, especially Dr. Khurram Shahzad Baig, Dr. Kashif Iqbal and Engr. Usman Asghar, without them it would not be feasible in the first place.

Whatever this document includes, is because to the great and wonderful intellect of the past, who dedicated their time and hard effort to make society a better place. Our heartfelt thanks to all the engineers and scientists who succeeded and those who did not. They may not be among us now, but their work lives on.

Abstract

Synthetic natural gas (SNG), that is a substitute of natural gas, is a commercially produced fuel from coal, biomass or solid waste. Due to its equivalent characteristics like natural gas, it can surrogate natural gas in terms of price, peak demands, and environmental concerns. The formation methods of SNG includes biochemical, electrochemical, and thermochemical pathway, of which thermochemical pathway has ascendency due to its high conversion rates, faster disposal time and less energy requirement. Due to its leading characteristics, thermochemical route seems to be most feasible process in Pakistan in terms of technical and economic viability while keeping in view of liquified natural gas import and solid waste growth rate. Therefore, thermochemical pathway was adapted in this report whereby detailed process flowsheet was composed that comprised of five sections.

Material balance analysis were made, on per hour basis, grounded on proposed capacity of plant, that was based on capacity of Gothenburg biomass gasification plant to avoid oversizing or under-sizing of equipment's. Furthermore, energy balance calculations were performed to deduce the overall energy requirements of the processing facilities.

The results from mass and energy balance were utilized to size the equipment in order to meet the desired outcomes. Besides process design, the vessel wall thickness required to sustain maximum stresses that vessel might be exposed to was also computed. Simulation of the proposed facilities of plant, was performed to replicate the plant in real word environment, is presented as a separate chapter in this report.

Following the design, an economic assessment of processing facilities was conducted to find payback period of initial investment. This project also took into account environmental regulations. A HAZOP analysis was conducted on adiabatic reactor, and the protection of the plant and employees was prioritized. At the end of the project, readers can find detailed references and appendices to assist them with various standard tables and charts.

Keywords: Solid waste gasification, Synthetic natural gas, Waste to energy, Solid waste management.

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CHAPTER # 01

INTRODUCTION

1. Introduction:

Synthetic natural gas or substitute of natural gas that consists of methane (CH_4) as its major constituent, is a commercially produced fuel from municipal waste or coal. It is a second-generation biofuel employing fourth generation combustion technologies in order to have similar characteristics as of fossil natural gas. Due to its similar properties like natural gas, it can be injected into natural gas infrastructure and transmitted to pipelines for end user. The carbon footprint of synthetic natural gas depends on the fuel source, as it can be low carbon or even carbon-free substitute of non-renewable fuels (hydrocarbon deposits).

According to Environmental impact assessment (EIA), the global energy demand will see a sharp rise of 50% by year 2050 with growing concerns of air quality, climate control and depletion of fossil fuels [1]. The share of renewable energy in the power market will be about 58.4% compared to 27.6% today [2]. The consumption of natural gas will rise to 31% by 2050 despite its limited resources. This paves the way for synthetic natural gas to fulfill the gas demands of the globe. As the supply of natural gas is restricted, synthetic natural gas is desirable when there is scarcity of natural gas in the region. Synthetic natural gas is more admirable than other renewable energy sources because of their intermittent operations, geographic limitations, and uncertainty of operations.

Recently, the process of utilization of municipal waste to produce SNG has become popular due to European climate law (June,2021) which sets an intermediate target of reducing greenhouse gas (GHG) emissions by 50% compared to 1990 levels (5,647 million metric tons of CO_2 equivalent) [3]. Prior to this technique, coal gasification was the main process for producing SNG. Multiple routes are available for synthesizing SNG from municipal wastes or biomass depending on the efficiency (of process) and economic feasibility of a region. The end users of Synthetic natural gas include,

- Electric Power
- Industrial Sector
- Commercial and Residential Sector

1.1. Properties of synthetic natural gas:

Synthetic Natural gas (also called Substitute natural gas) is a synthesized mixture of gaseous consisting primarily of methane in addition to various smaller amounts of trace gases like carbon dioxide, nitrogen. Synthetic Natural gas is colorless and odorless, so odorizes such as mercaptan, which smells like sulfur or rotten eggs, are commonly added for safety so that leaks can be readily detected.

1.1.1. Chemical properties:

Table 1.1: *Chemical properties of natural gas*

Chemical Properties	
Boiling point	-161.4 ºC
Melting Point	-182.5 ºC
Vapor Pressure	Very High
Vapor Density	0.7
Lower Explosive Limit (LEL)	5%
Upper Explosive Limit (UEL)	15%
Flash Point	-187.7 ºC
Flammability	Flammable Gas
Autoignition	537ºC

1.1.2. Physical properties:

Table 1.2: *Physical properties of natural gas*

Physical Properties	
Specific Gravity	0.422
Water Solubility	Slightly Soluble
Higher Heating Value	36.18 MJ/m^3
Wobbe Index	48.56 MJ/m^3

1.2. Reactions of product:

The major constituent of the synthetic natural gas is methane, which is produced by the methanation of syngas:

1.2.1. Methanation reaction:

The exergonic pathway in which CO_x is reacted with hydrogen to form methane is known as methanation.

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \quad \Delta H = -206\ KJ/mol \qquad (1.1)$$

The process of reacting CO_2 to hydrogen to form methane is known as Sabatier reaction.

$$CO_2 + 4H_2 \leftrightarrow CH4 + 2H_2O \quad \Delta H = -165\ KJ/mol \qquad (1.2)$$

1.2.2. Side reaction:

$$CO_2 + H_2 \leftrightarrow CO + H_2O \quad \Delta H = +41\ KJ/mol \qquad (1.3)$$

For selecting appropriate configuration for methanation system, the reactor performance is evaluated on the ranges of pressure, temperature, H_2/CO feed ratio. The highly exergonic CO methanation is accompanied by Sabatier reaction and water-gas shift reaction. The overall process is highly exothermic which requires an efficient heat removal system to clear the way for bio-methane production.

1.2.3. Natural gas reforming:

Steam reforming is a widely employed commercial pathway for producing hydrogen from natural gas with the overall process efficiency of 70-85 percent. [4]

Steam-methane reforming reaction:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \qquad (1.4)$$

Water-gas shift reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad (1.5)$$

During the final step CO_x and other impurities are removed through Pressure Swing Adsorption (PSA).

1.3. Industrial applications of synthetic natural gas:

1.3.1. For hydrogen production:

Natural gas (methane) is used as a precursor for producing hydrogen in a steam reforming process, whereby superheated-steam ((700-1000) ^{0}C and (3-25) bar) is reacted with methane in the presence of catalyst. Products of this endothermic reaction include hydrogen, carbon monoxide and carbon dioxide.

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \qquad (1.6)$$

Subsequently water-gas shift reaction takes place, making a way for pressure-swing-adsorption (PSA) to remove carbon-dioxide and other impurities.

1.3.2. Paper manufacturing:

Steam required for the manufacturing of paper and for driving paper mills is produced from power boilers which runs on natural gas.

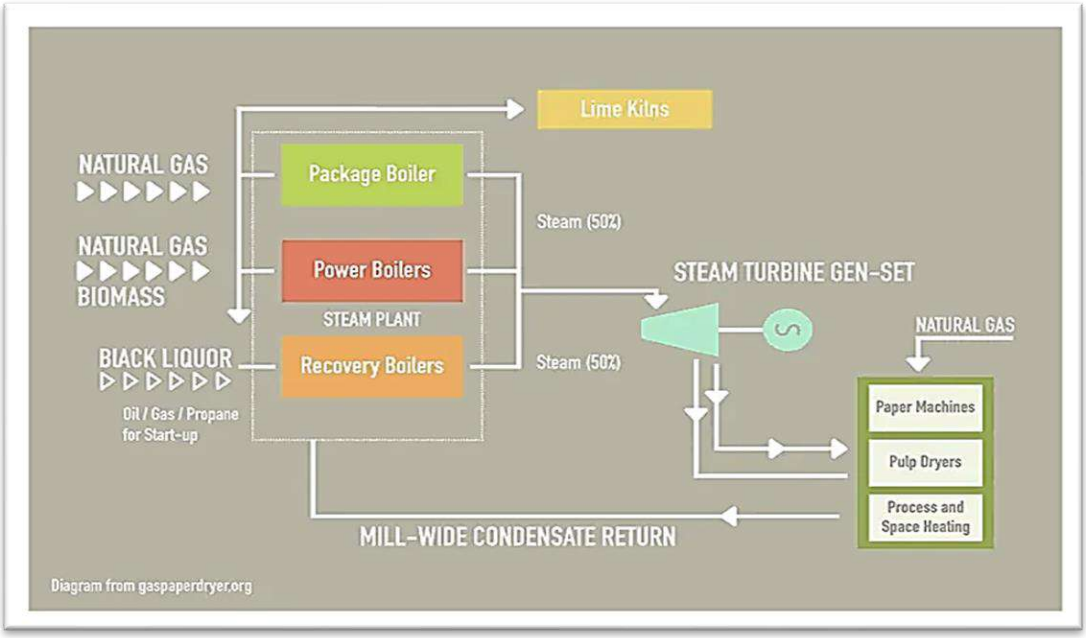


Figure 1.1: *Natural gas usage in paper industry* [5]

1.3.3. Fertilizer production:

Most of the nitrogen fertilizer is produced by a combination of natural gas and nitrogen from air [6]. Also, for the production of ammonia, syngas generation is required whose feedstock is natural gas [7].

$$CH_4 + 3H_2O \leftrightarrow CO + 3H_2$$

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

1.3.4. Power industry:

Natural gas is used by the power industry to generate electricity and thermal energy output. Moreover coal-fired power plants are now being replaced by gas-fired power plants due to net zero emissions by 2050 scenario.[8]

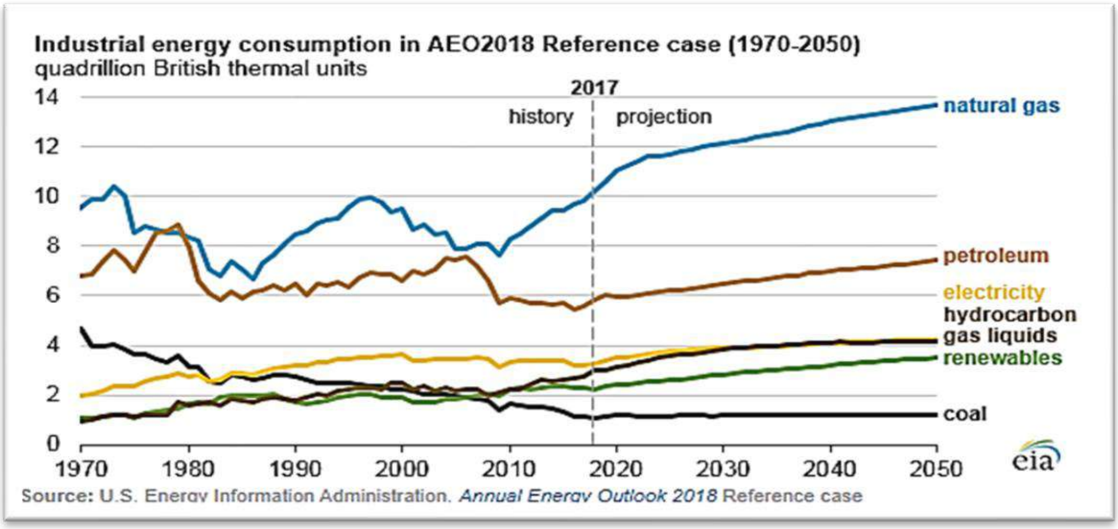


Figure 1.2: Projected industrial energy consumption of different fuels.(source: U.S. Energy Information Administration, *Annual Energy Outlook 2018*)

1.3.5. Handling, storage and safety:

The flash point of natural gas is -188 ^{o}C which makes it necessary to be handled or stored in a scrupulous manner.

- **Handling:**

Natural gas is a colorless, odorless, and highly explosive gas in which small amounts of odorants (mercaptans) are added for its characterization. It is lighter than air having specific gravity ranges from 0.55-0.87 due to variation in composition. Natural gas readily distributes itself in the atmosphere when leaked from a pipeline so care should be taken in installing ignition where natural gas is handled.

- **Storage:**

Large underground reservoirs are used for storage of natural gas to meet the seasonal demand of a region [9]. These underground storages include,

- Depleted gas reservoirs
- Aquifers
- Salt Caverns

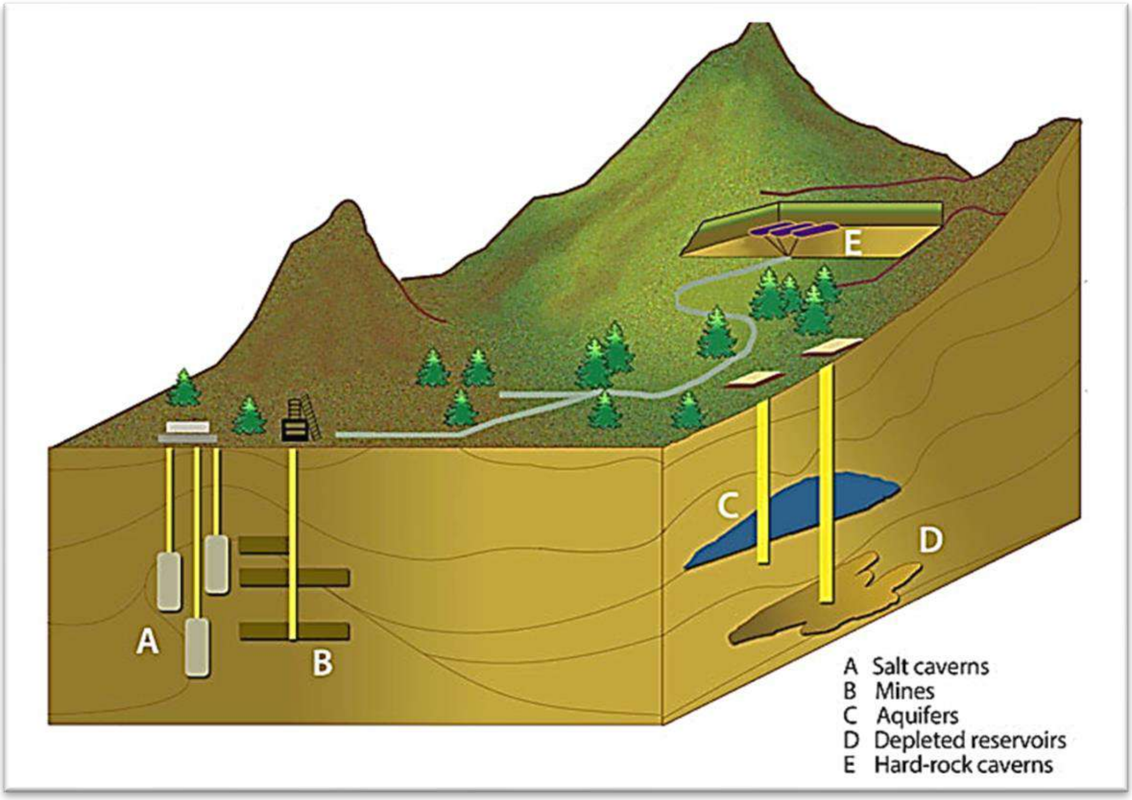


Figure 1.3: *Types of natural gas underground storage (source: PB-KBB, inc., enhanced by EIA)*

Sometimes natural gas is stored in liquified form (LNG) above the ground level in storage tanks ensuring low temperature for gas to be kept in liquid form.

- **Safety:**

Natural gas leaks are extremely dangerous and can be identified by a rotten egg odor. If one smells such an odor, then:

- Avoid touching or contacting the leak.
- Turn off all the flame sources and don't switch off or on the electrical appliances as it may create a spark.
- Locate yourself away from the leak.
- Avoid using the telephone or cell phone because static charges might ignite the gas.

- Don’t attempt to track down the leak.

1.1.5. Shipping of natural gas:

Natural gas is transported to regions, where pipeline natural gas cannot reach, in the form LNG. LNG is shipped or stored in extremely low temperature cryogenic tanks at a temperature of about -162 ºC. This makes the volume of a gas 600 times smaller than its gaseous form [10]. On the receiving port, LNG is re-gasified in order to be injected into pipeline distribution network. Liquified natural gas infrastructure includes:

- A gas pipeline from natural gas well.
- Liquefaction plant and storage facilities.
- LNG carrier
- Regasification terminal
- Pipeline distribution network.

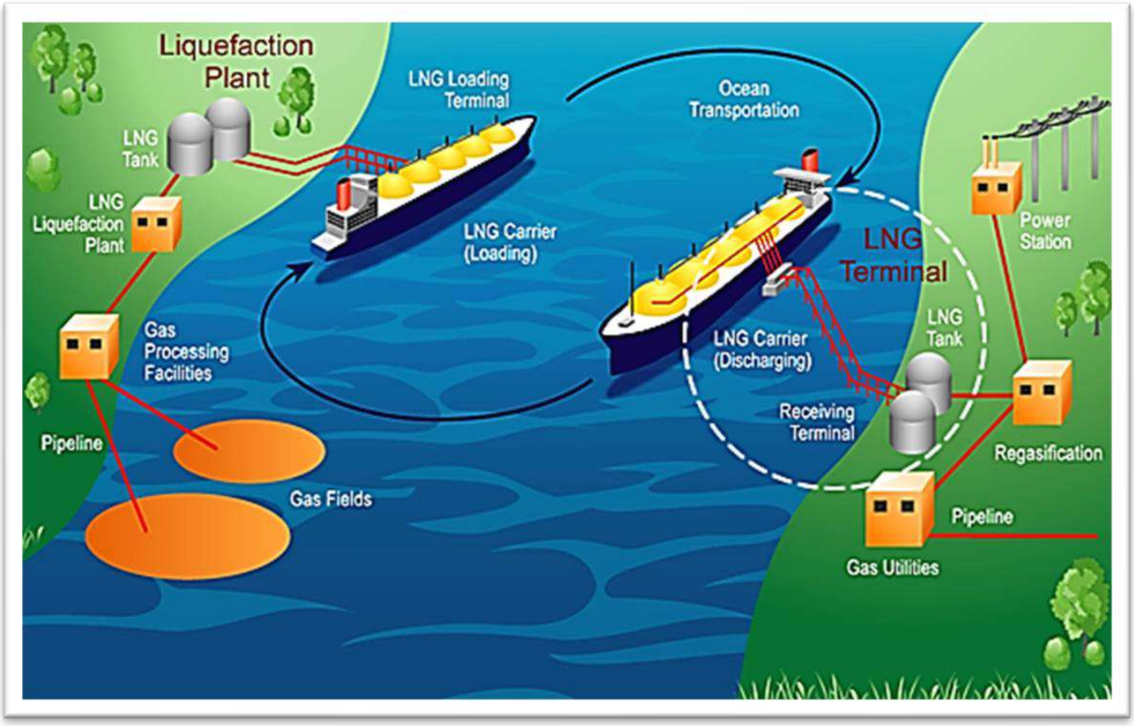


Figure 1.4: *Liquified natural gas exploration and production process (source: http://www.synfuels.com/)*

1.4. Project motivation:

To bridge a gap between energy demand and supply, Pakistan imports fossil fuels worth of US$ 12 million. Together with a Primary and imported energy supply, the carbon footprint in Pakistan has increased up to 208 Megatons with an average increase of 9% per year.

In Oct 2021, Pakistan set a conditional target of reducing its carbon footprint emissions by 50% in 2030 which means cumulative growth rate (CAGR) of renewable energy will see a sharp rise. Therefore, we have **opted for the manufacturing of SNG from biomass**. Moreover,

- It is carbon negative because it avoids the release of carbon dioxide into the atmosphere by converting CO_2 into fuel.
- Moreover, by recycling the unconverted CO_2 for formation of methane, it is possible to obtain a high concentration of synthetic natural gas, which is equivalent to commercial natural gas. This allows for gas from the municipal waste to become a potential source of alternative natural gas and can therefore have same applications as of fossil natural gas.

- It has relatively higher calorific value from other fuels except hydrogen. However, hydrogen is rarely used because of its incompatibility with the natural gas infrastructure, lack of storage and transportation.
- Synthetic natural gas can be low carbon or even carbon free alternative of natural gas, depending on the feed source.
- Depleting resources of fossil fuels thus allowing for fuel diversification.

1.5. Feasibility and current status:

The global gas market is anticipated to rise by 140 billion cubic meters from 2021-2025 according to gas market report. [11]

1.5.1. Feasibility:

Natural gas is a major player in fulfilling the global energy requirement, contributing about 25% of the total energy needs of the world [12].

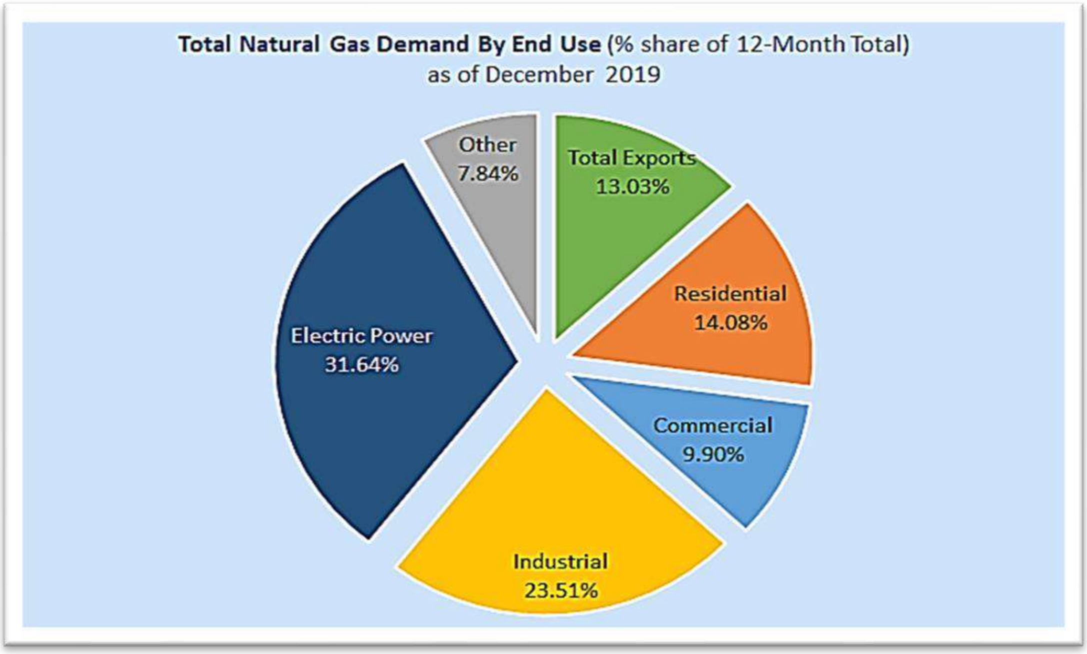


Figure 1.5: *Natural gas demand by end user (*source: Energy Information Administration, Bluegold Research estimates, and calculations)

The projected rise of natural gas in share of global energy mix is from 25% to nearly 30% in 2040 [13]. With urbanization, applications of natural gas in various sectors continue to rise due to its relative lesser carbon footprint than other non-renewable sources. The Compound annual growth rate (CAGR) of natural gas is expected to rise from 1.5% to 11.42% by the end of 2025 [14].

1.5.2. Status in the world:

The reserves of natural gas are one of the main causes of dominating world energy supply due to:

- Clean burning characteristics than other fossil fuels
- Relatively more economical than renewable energy options

Almost all countries of the world produce natural gas, with Russian federation having the upper hand. Natural gas fulfills 34% of the total energy demand in the United States, with France and Briton consisting of 16 and 37 percent of natural gas in their energy mix.

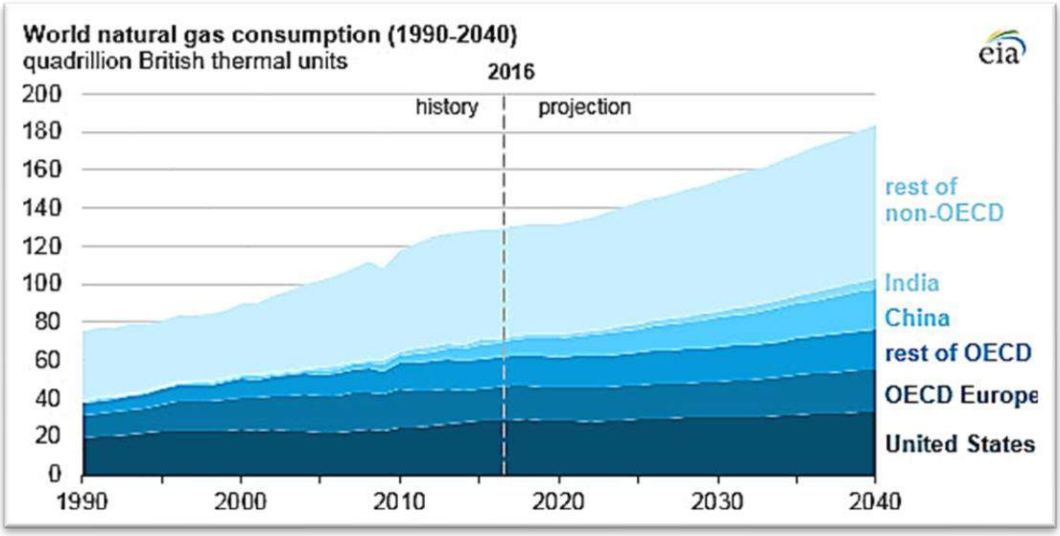


Figure 1.6: World natural gas consumption up to 2040 (source: U.S. Energy Information Administration, International Energy Outlook 2017)

1.6. Market assessment:

Limiting supply, high price of hydrocarbon deposits and government initiatives towards waste management and renewable fuels are driving force for synthetic natural gas market [15]. Moreover, due to ease in availability of raw materials and flexibility in composition adjustment, it can be used in chemical combinations for manufacturing different chemicals like acetic acid, ammonia, and Dimethyl carbonate. Thus, the development of chemical industries around the world increases the demand of SNG to utilize as fuel or lubricant. [16]

1.6.1. Global market:

The global size of Synthetic Natural Gas (SNG) Market size is anticipated to reach nearly from US$ 114.1 billion to 209.63 US$ billion by 2029 with the Compound annual growth rate (CAGR) of 4.5% during the forecast period. The most prominent growing demand of SNG is in the industrial sector where it is used as precursor for different applications.

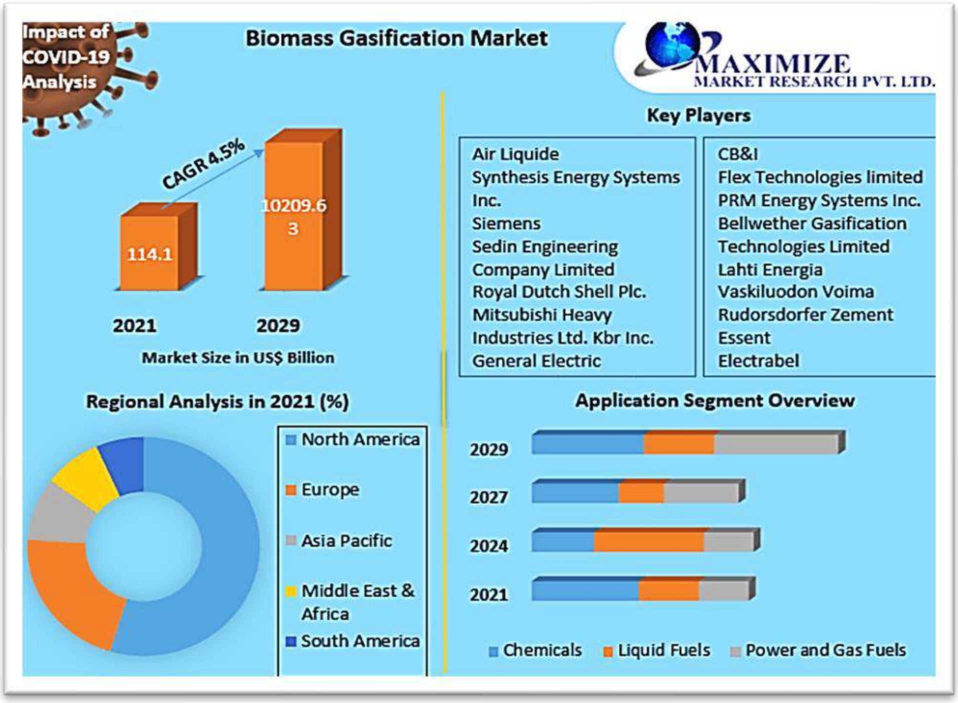


Figure 1.7: *Global SNG market (source: Veterinary Vaccines Market: Global Industry Analysis and Forecast 2029)*

Regional wise SNG market is segregated into Europe, Asia Pacific, North America, Middle East and Africa. North America market (including United States & Canada) is considered to be the dominating the other regional markets due to rise in demand and recent initiatives by the government for adoption of renewable and sustainable energy. Also, the Asia Pacific market is expected to rise at a considerable pace in the coming years.

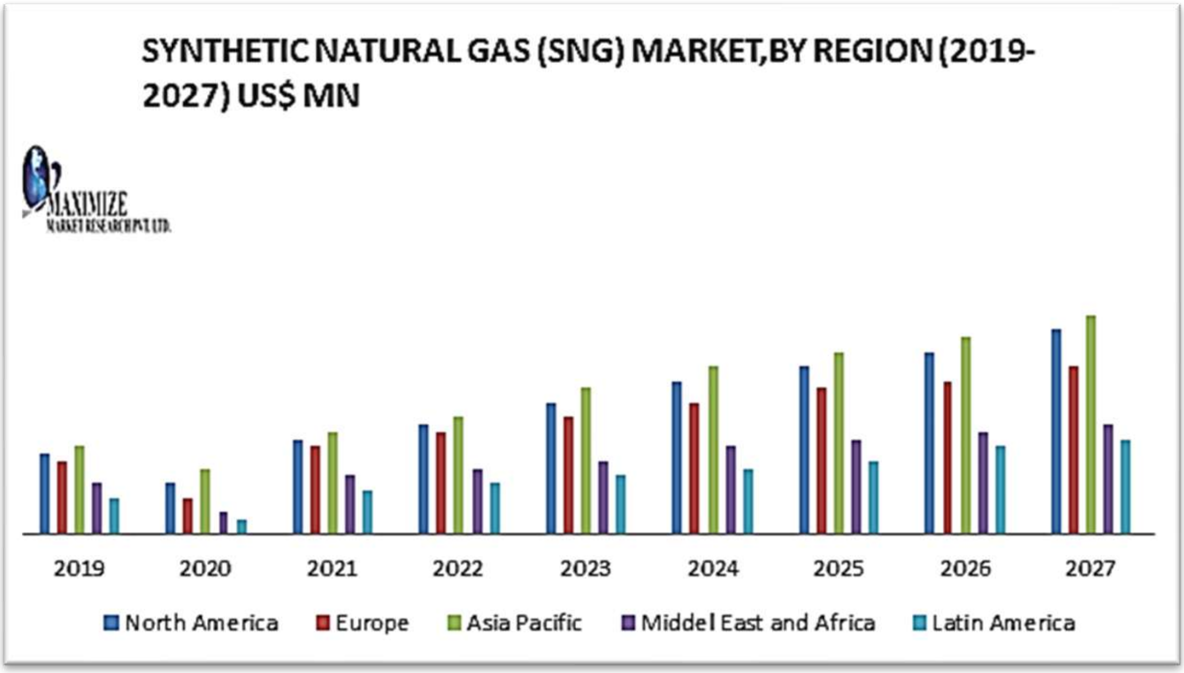


Figure 1.8: *Synthetic natural gas market by region (source: Synthetic Natural Gas (SNG) Market: Industry Analysis and 2019-2027)*

1.6.2. Production and consumption data:

Natural gas is the major commodity fuel in the world energy supply accounting for about 20 percent of total energy supply. Globally, the total volume of natural gas produced is 3.85 trillion cubic meters [17]. The following list gives the largest producer/consumer of natural gas,

Table 1.3: *Top consumer & producer of natural gas in the world*

Top Consumer & Producer of Natural Gas				
Rank	**Country**	**Consumption (billion cubic meters)**	**Production (billion cubic meters)**	**% Global Reserves**
1	United States	832	916	7
2	Russia	411	638	20
3	Iran	330	250	17
4	China	233.1	194	5
5	Canada	112	165	1

1.6.3. Pakistan's market of natural gas:

As a major fuel of domestic and commercial need, Natural gas contributes 20-30 percent of the total energy need of the nation. With its growing demand by the industrial and residential sector, natural gas resources are left for only 12 years with its current pace of consumption [18]. This means that reserve to production ratio (R/P) is only 12, else or otherwise more resources are found by unconventional means.

The domestic demand of natural gas in Pakistan is up to 6-8 billion cubic feet (bcfd) while production is only 4 bcfd which gives rise to a deficit of 2-4 billion cubic feet per day.

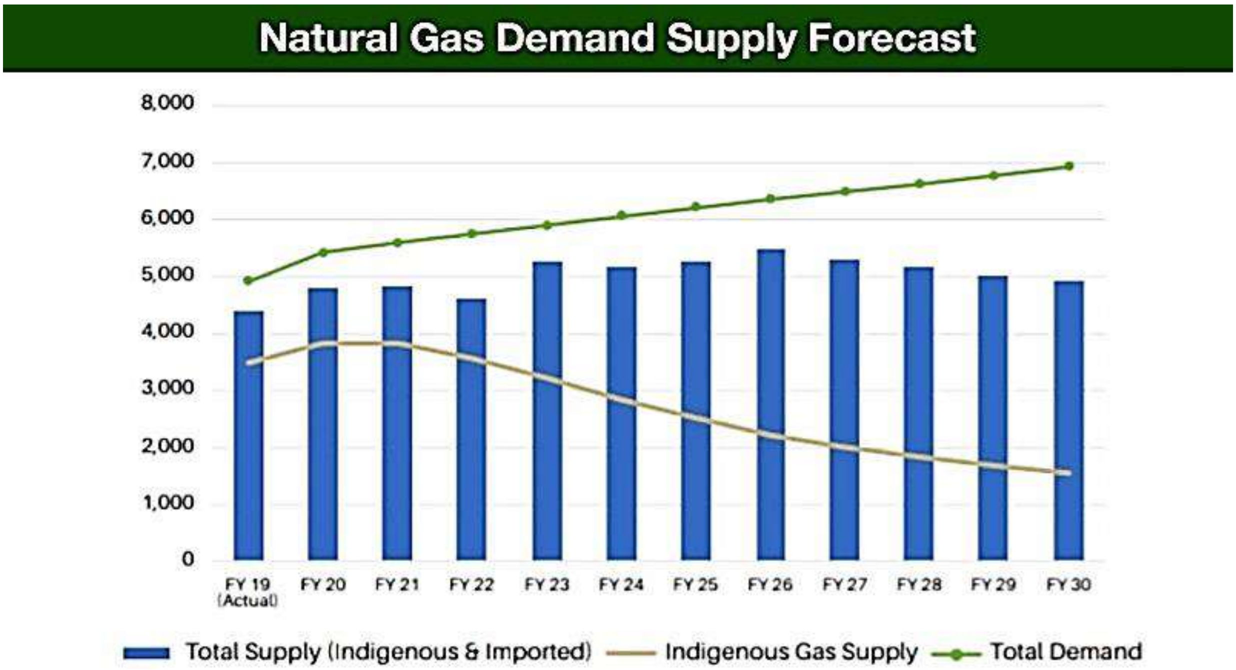


Figure 1.9: *Natural gas demand and supply forecast in Pakistan (source: OGRA)*

Province wise Gas consumption and production of natural gas is listed below,

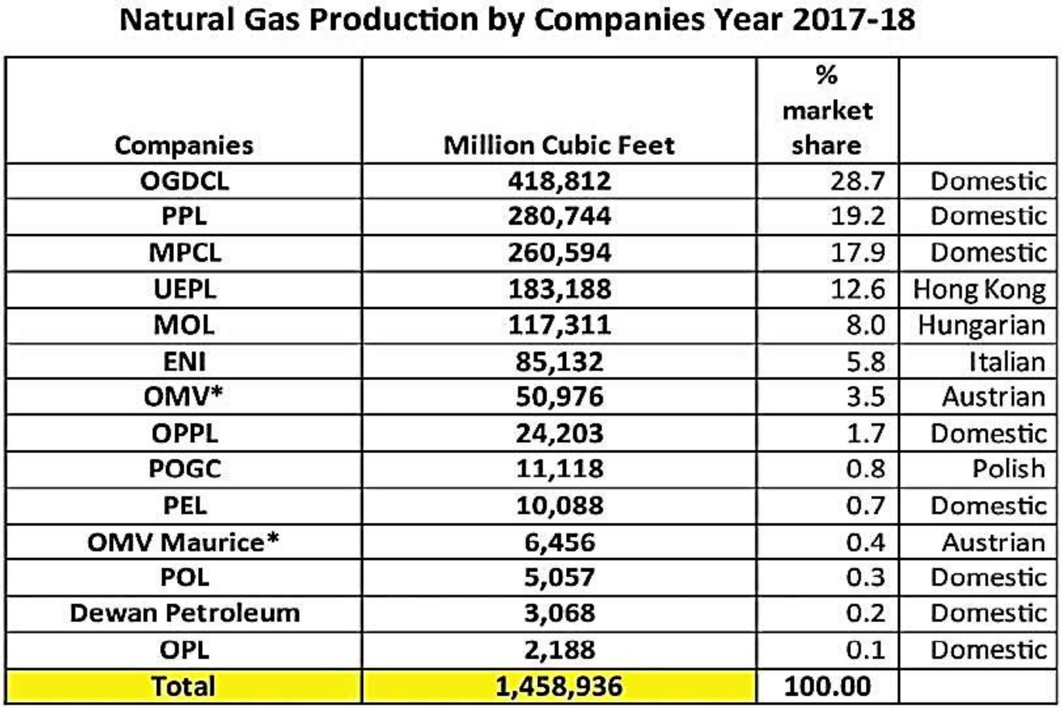
Table 1.4: *Natural gas province wise distribution in Pakistan*

Province	Production (mmcf)	Consumption (mmcf)
Sindh	943,644	515,004
Baluchistan	310,535	137,140
KPK	151,178	75,865
Punjab	53,580	729,468

The major player in the oil and gas market is Oil and Gas Development Corporation Limited (OGDCL) having market share of 30 percent, Pakistan petroleum limited (PPL) and Mari Petroleum with the market share of 19 & 18 percent. The rest of the share is filled by some domestic along with foreign companies.

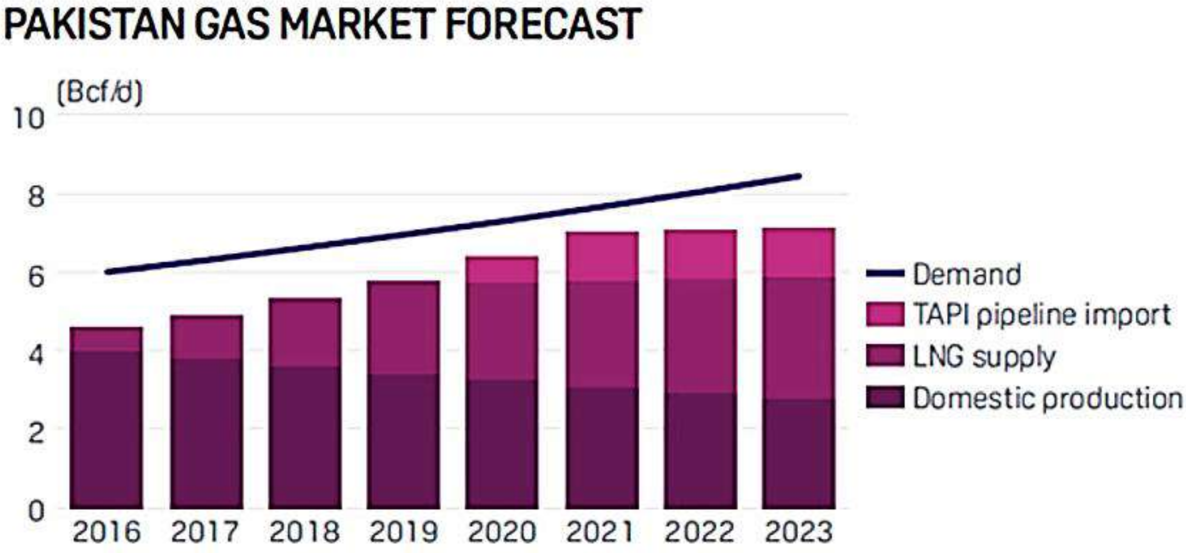
1.6.4. Future trends:

Table 1.5: *Oil and gas companies in Pakistan*



Natural Gas Production by Companies Year 2017-18

Companies	Million Cubic Feet	% market share	
OGDCL	418,812	28.7	Domestic
PPL	280,744	19.2	Domestic
MPCL	260,594	17.9	Domestic
UEPL	183,188	12.6	Hong Kong
MOL	117,311	8.0	Hungarian
ENI	85,132	5.8	Italian
OMV*	50,976	3.5	Austrian
OPPL	24,203	1.7	Domestic
POGC	11,118	0.8	Polish
PEL	10,088	0.7	Domestic
OMV Maurice*	6,456	0.4	Austrian
POL	5,057	0.3	Domestic
Dewan Petroleum	3,068	0.2	Domestic
OPL	2,188	0.1	Domestic
Total	**1,458,936**	**100.00**	



PAKISTAN GAS MARKET FORECAST

Source: Pakistan's Ministry of Petroleum and Natural Resources

Figure 1.10: *Pakistan gas market forecast*

According to Pakistan's ministry of Petroleum and Natural resources, the natural gas demand would continue to rise and to curb the growing demand LNG import would substantially increase while domestic production of natural gas would decline due to limited resources of fossil natural gas.

CHAPTER # 02

PROCESS SELECTION

2. Manufacturing processes:

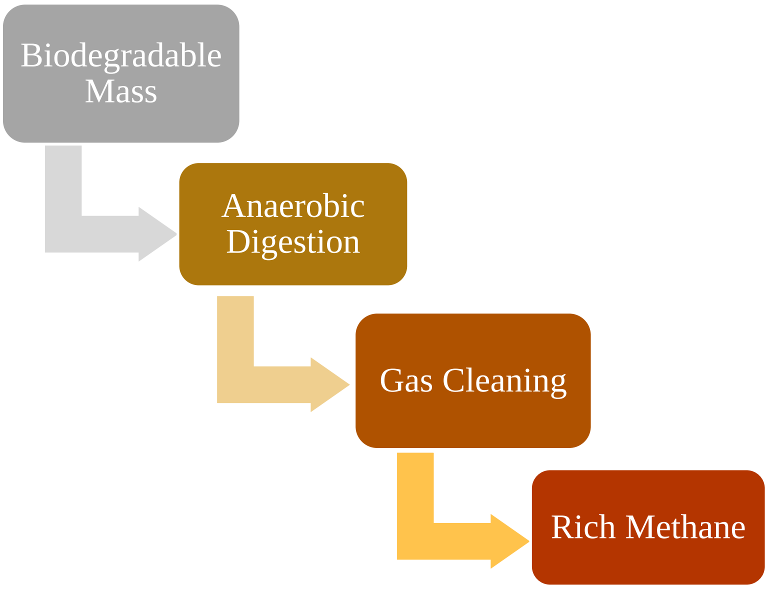
Synthetic natural gas from solid waste can be synthesize by three methods,[19] :

- Biochemical Pathway.
- Thermochemical Pathway.
- Electrochemical Pathway.

2.1. Biochemical pathway:

The biochemical path requires biodegradable feedstock to undergo anaerobic digestion for producing raw biogas. The raw biogas contains impurities including CO_2, H_2S, NH_3, BTX (Benzene, Toluene & Xylene), Siloxanes and dust particles which undergoes cleaning stages for producing a rich methane gas.

2.1.1. Process description:



2.1.1.1. Anaerobic digestion:

The biodegradable feedstock is fed to anoxic vessel where 4 types of microorganisms are fed for bio-fermentation. The four microorganisms include,

- Hydrolytic bacteria
- Ruminococcus
- Hydrogenotrophic methanogens
- Methanococcus Vannielli

Each microbe is specific for its function in digester. The four degradation steps of biodegradable material include,

- Hydrolysis
- Acidogenesis
- Acetogenesis and
- Methanogenesis

❖ **Hydrolysis:**

In hydrolysis, the complex organic matter consisting of proteins, carbohydrates, lipids and nucleic acid are broken down to monomers such as amino acids, fatty acids & sugars. This action is done by *hydrolytic bacteria* that secrete enzymes to convert carbohydrates, lipids and proteins. After the hydrolysis is completed, the products of hydrolysis diffuse into the cell membrane of acidogenic microorganisms. The optimum temperature and pH in hydrolysis process is 30-50°C [20]. The conversion in hydrolysis process is as follows;

$$Lipids \rightarrow Fatty\ Acids$$
$$Polysaccharides \rightarrow Monosaccharides$$
$$Protein \rightarrow Amino\ Acids$$
$$Nucleic\ Acids \rightarrow Purines$$

- **Acidogenesis:**

The monomers are further dilapidated by *Ruminococcus bacteria* into ammonia, hydrogen, carbon dioxide, alcohol and carbonic acid. Production of volatile fatty acids (VOFs), which consists of organic acids such as acetates, propionate and butyrate in a proportion of 75:15:10, also occurs in this step. Generally, if the VOFs are produced in greater amounts in acidogenesis process it inhibits the process of anaerobic digestion because the pH of digestor becomes too acidic which restrict the growth of microorganisms.

- **Acetogenesis:**

The VOFs produced during acidogenesis are consumed by acetogenesis microbes (for producing acetic acid) in order for methanogenesis to occur. Here the molecules are digested to further produce Hydrogen & Carbon dioxide.

- **Methanogenesis:**

During the last stage, products of acetogenesis are consumed by methanogenic bacteria to yield methane. This process is highly speculated process for which the microorganisms *methanococcus voltae* and *methanococcus Vannielli* may expose to aerobic environment which cause 99% of microbes to be killed. That's why this process is done in airtight chamber. The methane is produced by two processes,

1) Reduction of CO_2 with H_2 or by
2) Splitting of acetic acid to CO_2 and methane.

The following reactions occur in the methanogenesis process.

$$CO_2 + 4H_2 \rightarrow CH_4 + 2\,H_2O \tag{2.1}$$

$$\ldots\ldots \quad CH_3COO \rightarrow CH_4 + CO_2 \tag{2.2}$$

Typical gas composition form anaerobic digestion is,

Table 2.1: *Gas composition form anaerobic digestion.*

Component	Composition
CH_4	60%
CO_2	35%
N_2	1%
O_2	0.3%
H_2S	500 mg/m^3
Organic Sulfur	< 0.1 mg/m^3
Ammonia	0.7 mg/m^3
BTX	< 0.7 mg/m^3
Siloxanes	< 0.1 mg/m^3
Dust	> 5 micrometers

An Overall Reaction of anaerobic digestion is,

$$C_6H_{12}O_6 \rightarrow 3CO_2 + 3CH_4 \tag{2.3}$$

2.1.1.2. Gas cleaning:

Moisture from raw biogas is first condensed because of corrosion susceptibility of downstream equipment’s. Moisture can be removed by physical or chemical methods. The physical removal simply includes the condensation of water or by employing demisters. However, for fine tuning of biogas from water is to employ chemical methods including adsorption on activated carbon or silica. For H_2S removal two general methods are utilized,

- In-situ H_2S removal
- Downstream H_2S removal

In in-situ H_2S removal specialized microbes and iron chloride are inserted into the digester which reduces the hydrogen sulfide into elemental sulfur. The iron chloride then reacts with the elemental sulfur and forms FeS which easily be extracted from the system. However, this method doesn’t reduce the H_2S content to required level for downstream equipment. Downstream H_2S removal includes adsorption in Activated Carbon or ZnO bed, Chemical Scrubbing by MDEA with piperazine and Selexol Process. Also, Siloxane removal is done by absorption in organic solvents or adsorption on silica gel. The other trace components are eliminated altogether by activated carbon beds or CO_2 removal step. For CO_2 removal various chemical and physical methods are in practice,

2.1.1.2.1. Chemical methods:

- MEA (mono ethanol amine)
- MDEA (methyl di-ethanol amine)
- Chilled Ammonia
- DEA (di-ethanol amine)

2.1.1.2.2. Physical methods:

- Pressurized Water Scrubbing
- Selexol Process
- Rectisol Process
- Flour Carbon Capture
- Purisol Process
- Pressure Swing Adsorption
- Cryogenic Separation
- Membrane Separation.

After the gas cleaning stages, the maximum yield of methane occurs to be 92 % for single stage digestion process.

2.1.2. By product:

The by-product of this process is nutrient-rich digestate that can be used as soil amendment agent.

2.1.3. Limitations:

Biochemical pathway requires a much longer retention time for biogas production which is the main drawback. Also, the microbes are susceptible to deactivation (killed) if the solid waste contains some poisonous substance (ammonia rich). So, the feedstock for this process is only restrained to biodegradable rich nutrient material. Currently, state of the art biochemical plant reaches an efficiency of 54-57% with the potential of above 80% until the development of more efficient enzymes[19].

2.2. Thermochemical pathway:

The thermochemical pathway utilizes gasification technology and subsequent gas cleaning and methanation for producing synthetic natural gas. The scope of feedstock in this pathway is relatively wider due to gasification process because it can gasify almost anything [21]. The commercially available plants which falls under the category of thermochemical pathway includes;

- Gothenburg Biomass Gasification Plant (GOBI gas Sweden)
- Energy Research Center (Netherlands)
- Bio2G Project (Sweden)
- Güssing synthetic natural gas plant (Austria)

The Solid waste undergoes first pretreatment which makes the solid waste suitable for enhanced performance of gasifier. The gasifier converts the carbonaceous material from the solid waste into combustible non-condensable gases under the presence of gasifying agent. Of the many reactions occurring in gasifier, some are listed below.

$$C + \frac{1}{2} O_2 \rightarrow CO, \quad \Delta H^0 r = -111\ kJ/mol$$

$$C + H_2O \rightarrow CO + H_2, \quad \Delta H^0 r = +131\ KJ/mol$$

$$CO + \frac{1}{2} O_2 \rightarrow CO_2, \quad \Delta H^0 r = -161\ KJ/mol$$

The gasifier product (synthesis gas) also contains impurities namely organic & inorganic impurities. The synthesis gas is cleaned from such contaminants by hot gas cleaning or cold gas cleaning technology. After the gas cleaning step, the synthesis gas (mainly consisting CO, H_2, CO_2 & H_2O) is fed to methanation reactor where methane is synthesized by following exergonic reaction.

$$CO + 3H_2 \rightarrow CH_4 + H_2O, \quad \Delta H^0 r = -206\ KJ/mol$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O, \quad \Delta H^0 r = -165\ KJ/mol$$

The yield of methane varies from 94-98% by employing TREMP technology. The methane rich gas now undergoes water & CO_2 removal (under gas conditioning section) for meeting the standards required for natural gas grid injection. Overall process efficiency reaches up to 70% with the potential of reaching 75% by utilizing the waste heat recovered from exothermic reactions.

2.2.1. By-products:

The secondary product of this process is char which can be as a fuel and for making roads.

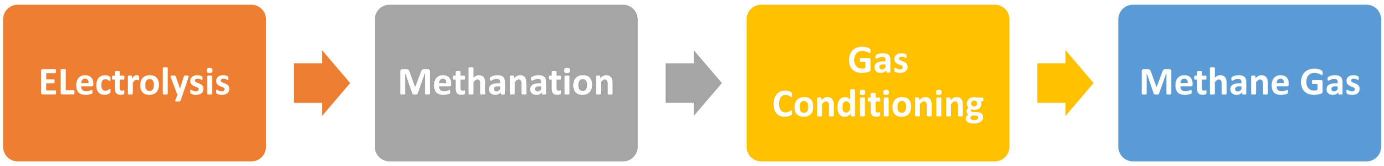
2.2.2. Limitations:

Temperature control is challenging task for methanation process which results in local hot spots inside the reactor. Also, the nickel-based catalyst applied for methanation is highly susceptible to sulfur poisoning. So, sulfur (in all forms) must be kept below the acceptable level for nickel catalyst.

2.3. Electrochemical pathway:

Electrochemical pathway utilizes electrolysis for producing hydrogen and carbon monoxide (syn gas) from water and CO_2. The synthesis gas then undergoes the same methanation process as described in thermochemical method. The yield of methane from this process is 98.4%.

2.3.1. Process description:



2.3.1.1. Electrolysis:

The excess electricity from the renewable or non-renewable resources is used to dissociate water and CO_2 (from market) to H_2, O_2 and CO. Oxygen is separated from the syngas (CO, H_2) and is sold as a by-product.

$$H_2O \rightarrow H_2 + \tfrac{1}{2}\, O_2$$
$$CO_2 \rightarrow CO + \tfrac{1}{2}\, O_2$$

Three different kinds of electrolysis are available to electrolyze this process.

- Alkaline Electrolysis
- Proton Exchange Membrane Electrolysis
- High Temperature Electrolysis

❖ **Alkaline electrolysis:**

Alkaline electrolysis (AEL) is the most mature electrolysis technique employing potassium hydroxide solution as electrolyte (25-30 wt.%). It occurs at temperature below 100 ⁰C, that's why it is not energetically favored because of subsequent downstream requirements of high temperature for methanation.

❖ **Proton exchange membrane electrolysis:**

PEMEL uses a polymer electrolyte for dissociation of water and carbon dioxide with the efficiency of 60-84%. These types of electrolytes are also operated al temp below 100 ⁰C but have higher current density (smaller area for same power output as AEL). Moreover, PEMEL is more suited for high pressure applications due to its compact design.

❖ **High temperature electrolysis:**

High temperature electrolysis (HTEL) or solid oxide electrolysis (SOEC) are operated at temperatures up to 700-1000 ⁰C resulting in less energy requirements for downstream methanation process. This type of electrolysis employs solid oxide as electrolyte while operating on a thermo-neutral voltage resulting in a constant electrolysis temperature. Thermo-neutral voltage is ratio of heat produced by the cell to the heat consumed by the electrolysis. So, no constant cooling of cell is required during electrolysis in SOEC while the other two technologies are operated above thermoneutral voltage resulting in constant cooling requirements because of rise of temp during electrolysis. Moreover, the power input of SOEC is relatively smaller than it's competing technologies due to,

- Faster reaction kinetics due to high temperature
- Lower internal resistance at high temperatures.

However, this technology is still in development scale causing unpredictability of its performance.

Now, the synthesis gas from electrolysis is compressed to methanation inlet pressure because higher pressure favors the production of CH_4 for this reaction.

2.3.1.2. Methanation:

The hydrogenation of carbon oxides for formation of methane is known as methanation. The methanation reaction is thermodynamically favored al low temperatures and high pressures [22].

$$CO + 3H_2 \rightarrow CH_4 + H_2O, \qquad \Delta H^0 r = -206\ KJ/mol$$
$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O, \qquad \Delta H^0 r = -165\ KJ/mol$$

The catalyst used for this process is Nickel based on Alumina support to enhance the specific surface area of active material. The first reaction is known as reverse steam reforming reaction while the second reaction is Sabatier reaction. Both the reactions are highly exothermic requiring external cooling to thermodynamically favor the product side of reaction.

2.3.1.3. Gas conditioning:

The product gas now is upgraded in terms of CO_2 or H_2O for adjusting its specific gravity and wobbe index. The same CO_2 separation technologies are applied as previously mentioned for biochemical route while H_2O is removed by cooling and condensing the product gas. The overall process efficiency is 54-60% having potential of above 70% when employing SOEC electrolysis [19].

2.4. Comparative study of different routes:

Table 2.2: *Comparative study of different routes*

	Biochemical	Thermochemical	Electrochemical
Pressure (bar)	32	**5**	33
Temperature (^oC)	60	**250-700**	800
Methane Yield (%)	92	**94-98**	98.4
Advantages	Low processing temperature Lowest production cost (8 €ct)/Kwh$_{SNG}$	**Effectively applied to any biomass feedstock** **Less reaction times.** **High SNG output (380 MW)** **Low production cost (11.3 €ct)/Kwh$_{SNG}$**	Higher methane yield.
Drawbacks	High retention time Only for specific feedstock Lowest SNG output (5.6 MW)	**High processing temperature.**	High power input Low SNG Output (88.5 MW) Highest Production Cost (27.3 €ct)/Kwh$_{SNG}$

2.5. Process selection:

The most feasible process for producing synthetic natural gas from solid waste is thermochemical process due to:

- Conversion rates and feasibility is much higher than biochemical process and thermochemical process because of faster disposal time and less power input (compared to electrochemical process) [21].
- Overall high process and energy efficiency [23].
- Greater potential of installing a commercial size plant due to well-developed gasification technology and its ability to tolerate diverse feedstock.
- Higher volume reduction of solid waste as compared to other competing processes.

2.6. Feedstock, its availability & supply:

2.6.1. Feedstock:

Municipal solid waste is the selected feedstock for producing synthetic natural gas because of its wide availability in Pakistan.

2.6.1.1. Municipal solid waste:

Municipal solid waste often known as trash or rubbish is a daily waste generated or discarded by the people or waste that is collected by the local municipalities of an area. The composition of municipal solid waste can vary slightly from region to region. The sources of municipal solid waste include commercial, institutional, residential and industrial. Most of the municipal solid waste in developed countries ends up in recycling stations, landfills or thermal processing plants. The thermal processing plants include incinerators, gasification and pyrolysis. The projected waste generation by region is shown below,

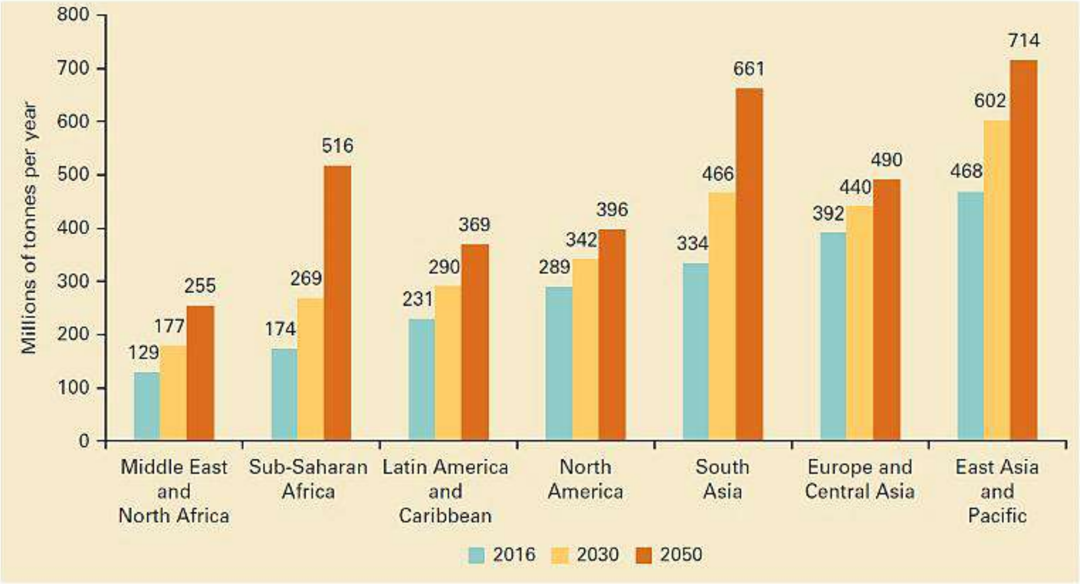


Figure 2.1: *Projected waste generation by region (source: World Bank)*

Moreover, municipal solid waste is also treated biologically involving composting (Aerobic Digestion) and Anaerobic Digestion. This treatment is done to transform solid waste into that form that is utilizable or easy to handle.[24]

2.6.2. Availability in Pakistan:

According to international trade administration (ITA), Pakistan creates about 49.6 million tons of municipal waste annually with the growth rate of 2.4 percent per annum [25]. Most of the solid waste in Pakistan is either sent to landfills, buried on vacant sites or incinerated (creates Furans and Dioxins). Only 70-80% of the solid waste is collected by primary and secondary collectors. Primary collection includes carts, donkey pulls while secondary collection is by cars and trucks.

Landfill sites are places where waste is isolated from the environment and is decomposed either chemically or biologically. The country’s biggest city has only 3 landfills while Lahore has only 2. Plans are underway for building landfill sites in major cities of country. Meanwhile in Punjab, Lahore is the only city having proper waste management and disposal system. For Sindh, Asian Development bank (ADB) has approved $400 million in 2019 for improving waste management infrastructure. In KPK, water sanitation services Peshawar (WSSP) is drafting to build a landfill site. Baluchistan province has not any notable infrastructure for waste management. The solid waste generation in major cities of Pakistan is shown below,

Table 2.3: *Solid waste generation in major cities of Pakistan*

City	Municipal Solid Waste Generation (Tons/Day)
Karachi	16,490
Lahore	7,688
Faisalabad	5017
Rawalpindi	4,448
Hyderabad	3,973
Multan	3,679
Gujranwala	3,479
Sargodha	3,070
Peshawar	2,047
Quetta	715

Composition of municipal solid waste of Lahore city is,[26]

Table 2.4: *Composition of MSW of Lahore city*

Serial No.	Description	Weight (%)
1	Paper	5.04
2	Glass	2.19
3	Ferrous Metal	0.02
4	Non-Ferrous Metal	0.47
5	Film Plastic	12.94
6	Rigid Plastic	5.55
7	Organics	67.02
8	Textiles	1
9	Others	5.77
Total		100

2.6.3. Feedstock suppliers:

Major waste collection companies in Pakistan are;

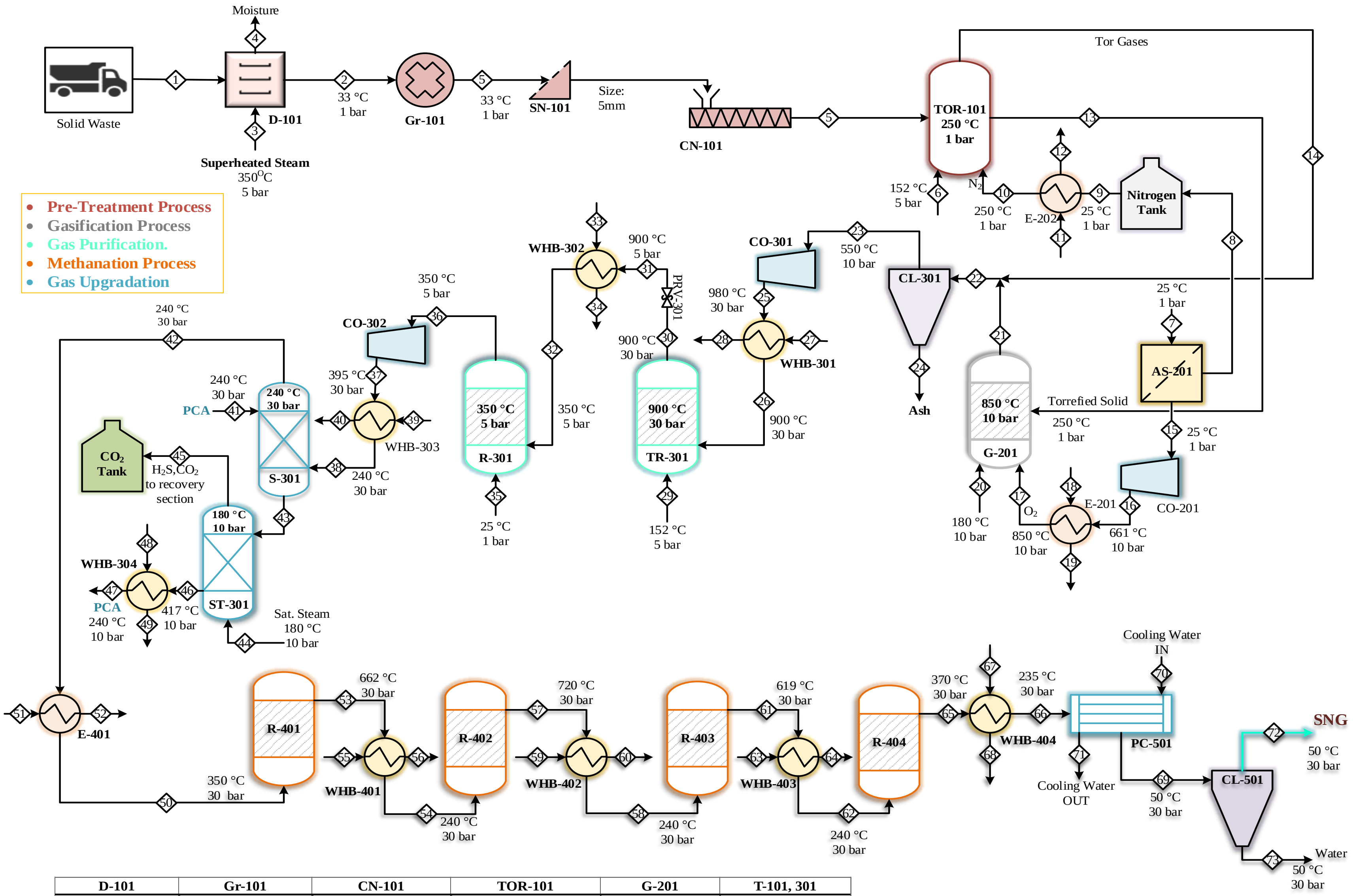
- Lahore Waste Management Company.
- Lahore Waste Buster.
- Farsa Waste Busters.
- Rawalpindi waste management company.
- Multan waste management company.
- 3R & Incinero Waste Management Company Lahore.
- Sindh Solid Waste Management.
- Faisalabad waste management company and many more.

Lahore waste management company (LWMC) has average collection capacity of 2500 tons of solid waste/day while Faisalabad waste management company can collect waste up to 880 tons/day [27]. So, it seems that abundant amount of raw material is available in Pakistan for making such process (producing SNG from solid waste) sustainable.

2.7. Detailed process description:

The process is divided into the following major steps.

- Pretreatment of raw material.
- Gasification of solid waste.
- Gas purification.
- Synthetic natural gas production.
- Gas conditioning.



D-101	Gr-101	CN-101	TOR-101	G-201	T-101, 301
Dryer	Crusher	Conveyer	Torrefaction	Gasifier	N_2, CO_2 Storage Tank
AS-201	**S-301, ST-301**	**CL-301, 401**	**TR-301**	**R-301**	**R-401, 402, 403, 404.**
Air Separating Unit	Scrubber, Stripper	Cyclone	Tar Reformer	WGS Reactor	Methanator

Figure 2.2: *Process flow diagram*

2.7.1. Pretreatment of raw material:

Pretreatment or pre-conditioning of raw material is done in order to meet the required specs of feed for producing SNG. Without Pretreatment solid waste has,

- Low energy density.
- Poor combustion attributes.
- Low calorific value.
- High moisture content and,
- High hydrophilicity and hence high transportation cost.

The pretreatment section is involved.

- Drying,
- Crushing and
- Torrefaction.

2.7.1.1. Drying:

The feedstock initially contains approximately 50 wt.% moisture content (from proximate analysis) which must be reduced well below 20 wt.% in order have high content of carbon monoxide [28]. Drying increases the hydrophobicity of waste by eliminating bound and unbound water. Thus, reducing its water absorption properties. Due to increased hydrophobicity, solid waste can be stored for increased period [29]. Different types of dryers are used in which the drying medium may be steam driven, air driven, vacuum driven, or freeze drying.

2.7.1.2. Crushing:

The dried solid waste is crushed and screened to 5mm particles. Screen is installed to have uniform particle size entering the reactor and thus having same space time resulting in high performance. This is due to decreased diffusion resistance of smaller particles and hence enhancing the total syngas yield. [30]

2.7.1.3. Torrefaction:

Transforming raw waste into high grade solid fuel (bio-coal) is known as torrefaction. Torrefaction, also known as mild pyrolysis (200-300 ºC), is a thermal pretreatment of solid waste in order to alter its chemical properties for increasing efficiency of advanced thermochemical processes such as gasification or pyrolysis [31]. Torrefaction may be classified into

- Light Torrefaction (200-235 ºC)
- Mild Torrefaction (235-275 ºC)
- Severe Torrefaction (275-320 ºC)

The product yields of torrefaction depend on operating temperatures, residence time and heating rates. Torrefaction leads to,

- Increased energy density.
- Increased fixed carbon content, thus increasing heating value.
- Increases syngas yield & quality.
- Increased gasification efficiency.
- Reduced H/C, O/C and tar content.
- Reduced formation of agglomerates at high temperatures in gasifier.
- Reduced moisture content.

2.7.1.3.1. Torrefaction process:

The raw solid waste contains lignocellulosic mass (hemicellulose, cellulose and lignin) which gets degraded on increasing temperature. The effect of rise in temperature on proximate analysis of solid waste is,

- Volatile matter and moisture content is removed due to the degradation of hemicellulose and cellulosic content. [32]
- Fixed carbon is increased which results in higher heating value at increased temperatures due to the only presence of lignin content. Lignin content contains more C-C bonds than C-H or C-O bonds, so calorific value is increased at high temperatures.
- Likewise, an increment in ash content is seen at high temperatures.

The volatile matter degrades at high temperatures due to presence of low boiling point organic compounds. This results in reduced mass of torrified product relative to its original sample. Similarly, the effect of increased temperature on elemental analysis of solid waste is,

- High temperature results in increased carbon content due to elimination of oxygen and hydrogen containing compounds.
- Oxygen compounds are removed due to cracking of oxygen containing functional groups to generate carbon oxides.
- As a result, O/C ratio and H/C ratio decreases which results in high calorific value [33].

The **calorific value** of torrified solid waste was increased from (6.3-10.9) MJ/Kg to (17-36) MJ/Kg.[29] Moreover, torrefaction results in 7% more H_2 and 20% more CO in syngas [34]. Overall degradation of substances in torrefaction can be demonstrated as:

Deoxygenation > Dehydrogenation > Decarbonization

The general expression of torrefaction can be written as,

$$Solid\ waste \ \rightarrow \ Torrefied\ Product \ + \ Volatiles$$

The solid, liquid and gaseous yield of torrefaction depends operating temperatures. Due to rise in temperature, the liquid and gas yield increases which terminates the purpose of torrefaction. So, an optimum increase in temperature is required where solid product distribution is maximum, and fluid is minimum. At 250 °C & residence time of ≤ 30 mints, the solid yield is above 85 % [29].

2.7.2. Gasification of solid waste:

Gasification (partial oxidation) involves conversion of carbonaceous materials in solid waste to synthesis gas in the presence of gasifying agent. The solid waste is converted into gaseous mixture through devolatilization and partial gasification of char. The char product can be used separately as a fuel or for making roads.

Gasification is more universal than pyrolysis due to its higher syngas yield [35]. Generally, the selection of thermochemical technology is dependent on the product. If end product is gas, then gasification would be a suitable technology. However, if the product is liquid fuel or solid fuel then pyrolysis is preferred. Moreover, the final product compositions of these thermochemical technologies are,

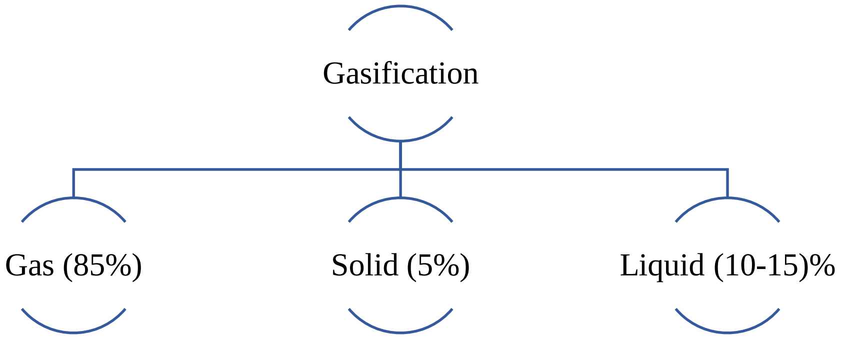


Figure 2.3: *Gasification product yields*

For Fast Pyrolysis,

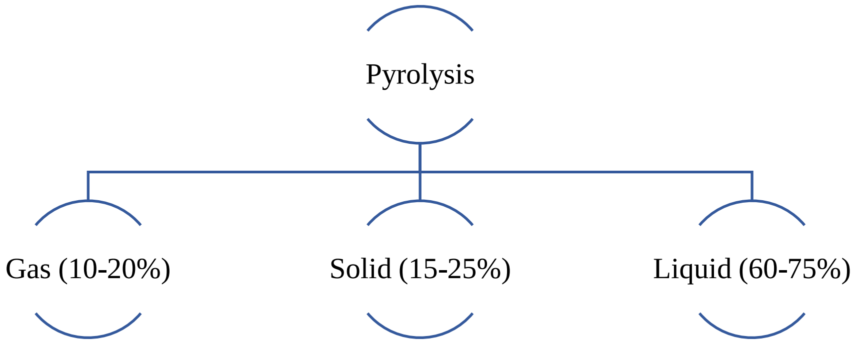


Figure 2.4: *Fast pyrolysis product yields*

2.7.2.1. Gasification technologies:

Based on energy supply, gasification technologies are divided into,

- Direct and,
- Indirect gasifier.

2.7.2.1.1. Direct gasifier:

In direct gasifier, the fuel is fed directly into the gasifier while steam as a gasifying agent interacts with air or oxygen to produce syngas. The heat required for endothermic gasification process is supplied through oxidation reactions inside the gasifier. Having this, only single reactor is used for gasification process. However, the dilution of syngas with N_2 occurs if air is fed. So, air separating unit (ASU) is installed before the gasifier for nitrogen free syngas.

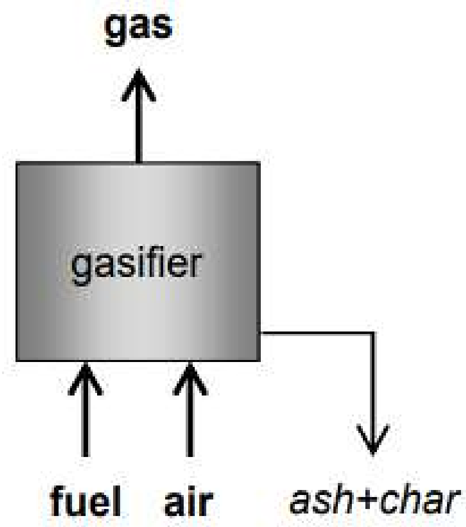


Figure 2.5: *Direct gasification*

2.7.2.1.2. Indirect gasifier:

In indirect gasifier, gasification occurs in the absence of gasifying agent, thus requiring an external heat source for gasification reactions to occur. The char along with bed material from the gasifier is fed into combustor where it combusted to produce flue gas, heat and ash. The bed material absorbs heat from the combustor and is recycled into the gasifier to sustain the reactions occurring in the 1st reactor (gasifier). The products of gasifier are synthesis gas, which is free from nitrogen, and char which is again circulated through the combustor and recycled back to gasifier. Such a configuration, involving gasifier (1st reactor) and combustor (2nd reactor), is usually complex where a bed material is used to exchange heat between two processes. Moreover, these types of gasifiers are usually operated when air is used as gasifying agent or oxygen is fed in the form of air.

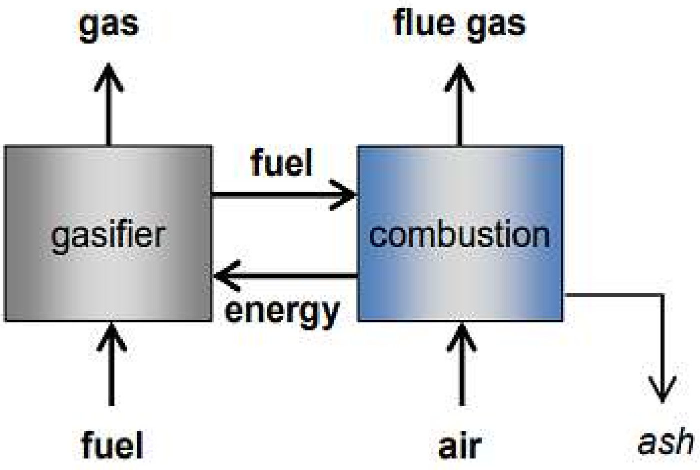


Figure 2.6: *Indirect gasification*

2.7.2.2. Gasifier types:

- Fixed bed,
- Fluidized Bed and,
- Entrained Flow.

2.7.2.2.1. Fixed bed gasifiers:

The gasifier in which the bed of catalyst is fixed between the packing supports is known as fixed bed gasifier. These are further divided into updraft and downdraft fixed bed gasifier.

Updraft gasifier works by allowing the gasifying medium to counter currently contact with the fuel from the top resulting in synthesis gas which is drawn from the top of the gasifier. While the slag or ash is drawn from the bottom of the gasifier. The fuel or solid is converted into synthesis gas in four sections of updraft gasifier,

- Drying
- Pyrolysis
- Reduction and
- Oxidation

The tar resulting from pyrolysis section is carried upwards due to the high velocity of syngas, thus resulting in high tar content of product gas. However, the feedstock or fuel is preheated due to the sensible heat exchange between the syngas and the feedstock [36].

In downdraft gasifier, both the carbonaceous material and the gasifying agent is introduced through the top while syngas is drawn from the bottom. The highest operating temperatures ranges from 1000-1050 ^{0}C which allows the thermal cracking of tars. However, both these types of gasifiers are used for small scale plants [37].

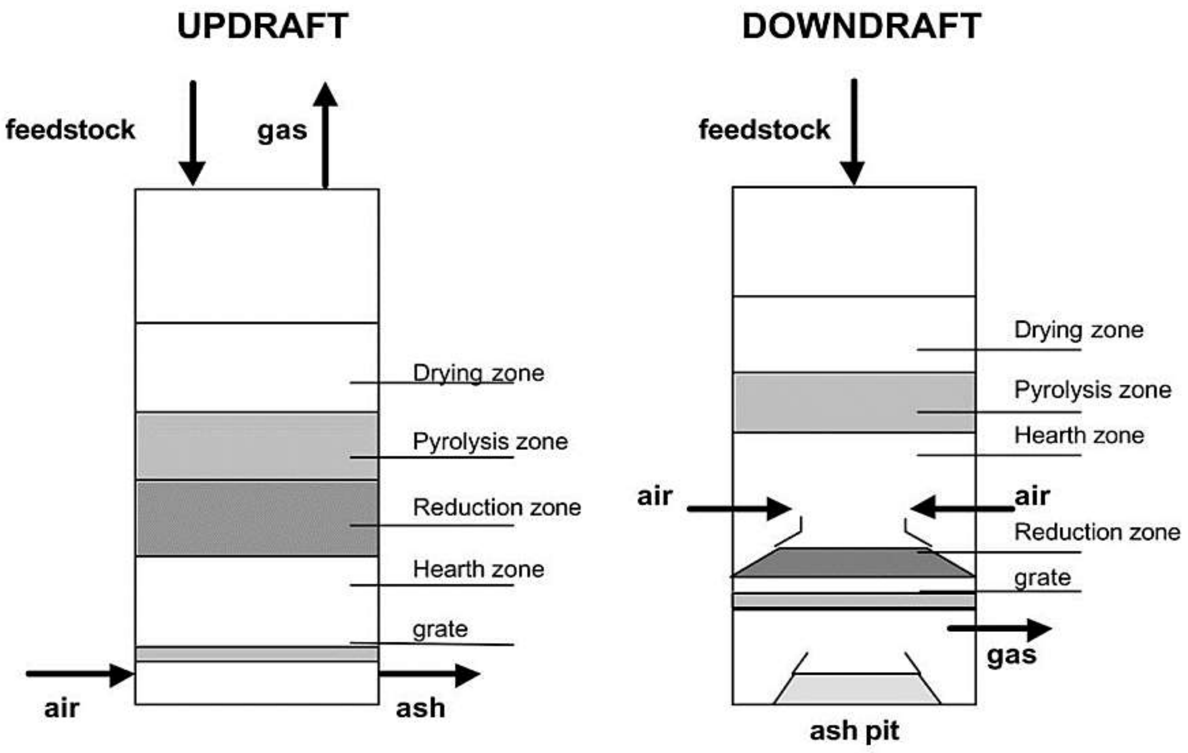


Figure 2.7: *Updraft and downdraft gasifiers*

2.7.2.2.2. Fluidized bed gasifiers:

Fluidization is known as the suspension of solid particles by the action of fluid. In fluidized bed gasifiers the catalyst medium along with some feed particles are suspended by the gasifying agent resulting in greater contact between the reacting phases. Due to fluidization, these types of reactors can be operated isothermally due their easy heat removal and good temperature control [38]. Moreover, these gasifiers can accept diverse feedstock including high ash content.

They have efficiency about 5 times of fixed bed gasifier and are operated at temperatures between 700-900 ºC with highest limit set by ash softening point which results in agglomerates formation inside the gasifier. Fluidized bed gasifier is classified as,

- Bubbling fluidized bed
- Circulating fluidized bed

In **bubbling fluidized bed gasifiers (BFB)**, the gasifying agent velocity is around 2-3 m/s causing only expansion of the bed materials without exceeding their terminal velocity (velocity if exceeded causes carryover of the particles from the gasifier) [37].

In **circulating fluidized bed gasifier (CFB),** the up-flowing velocity of gasifying agent is 5-10 m/s which results in entrainment of solid catalyst. The entrained catalyst is then captured and recycled back to gasifier through cyclone action.

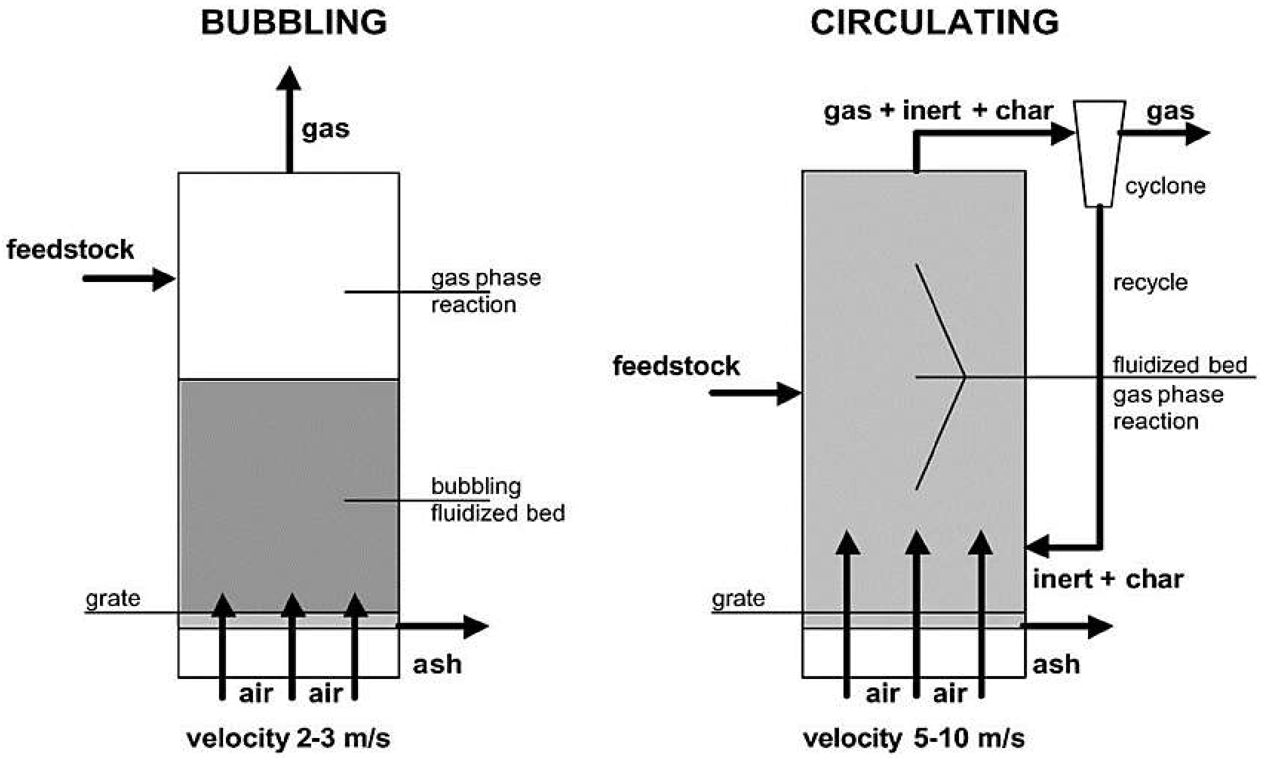


Figure 2.8: *Bubbling & circulating bed gasifiers.*

2.7.2.2.3. Entrained flow gasifiers:

Entrained flow gasifiers are comparatively new having relatively higher process efficiency with the requirement of pulverize feedstock. They are operated at extremely high temperature (1000-2000 ºC) which results in complete removal of tar. These are usually,

- Top-fed
- Side-fed

In top-fed gasifier, finely divided particles along with gasifying media is fed from top in the form of jet. High temperature product gas is withdrawn from the side while slag is accumulated on the bottom of reactor. While in the side-fed gasifier, pulverize fuel and gasifying agent is fed from the lower part through nozzle which results in appropriate mixing of fuel. Product gas is withdrawn from the top while slag collected from the bottom.

Table 2.5: *Gasifier technologies*

Gasifier Technologies			
	Fixed Bed	**Fluidized Bed**	**Entrained Flow**
Product gas temperature	Low (430-650 ºC)	Moderate (700-1040 ºC)	High (1230-2000 ºC)
Oxygen demand	Low	Moderate	High-capacity ASU
Steam used	High	Moderate	Low
Internal moving parts	Yes	No	No
Feed size	< 100mm	< 50mm	< 1.5mm

- Operating temperature & pressure of gasifier: 850 ºC & 10 bar.
- Catalyst used: Calcined dolomite.
- Conversion: 90% [39]

2.7.3. Gas purification:

The raw synthesis gas from the gasification is addressed to downstream section of gas cleaning which comprises of,

- Cyclone separator
- Tar reformer
- Water-gas shift
- Sulfur and CO_2 removal

2.7.3.1. Cyclone separator:

The syngas containing particles enter the cyclone at a tangential velocity causing centrifugation which results in particulate removal with an efficiency of 99%. Since cyclone has no moving parts, the highest temperature of the cyclone is constricted by material of construction. The particles from cyclone can be combusted in a combustion chamber thus providing heat where necessary in the process.

2.7.3.2. Tar reformer:

Tars are complex aromatic hydrocarbons that condenses at low temperatures causing clogging of downstream equipment's, forming tar aerosols & long chain polymeric hydrocarbons. These usually results due to the decomposition of lignocellulosic biomass during the pyrolysis step. Typically tar contains 3 ring aromatic hydrocarbons, 4 rings aromatic hydrocarbons, phenolics compounds and naphthalene. Usually, tars are removed by hot gas cleaning or cold gas cleaning technology.

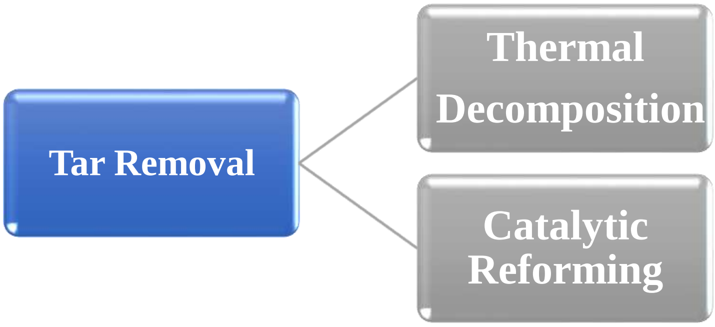
- **Cold gas cleaning:**

All the wet scrubbing technologies which involve solvents for tar removal are known as cold gas cleaning methods. These methods are usually ineffective because the synthesis gas has to be cooled down to 100ºC which is thermodynamically inefficient. Moreover, due to these methods tar disposals becomes an issue.

- **Hot gas cleaning:**

Cleaning of synthesis gas above 260ºC is known as hot gas cleaning [40]. Hot gas filters are usually employed when syngas can be processed at higher temperatures up to 650ºC, without damaging downstream equipment, and cooling of syngas is not energetically favored.

Tar removal under hot gas cleaning can be done in two ways;



Thermal decomposition requires temperatures above 1000ºC for decomposing tars into syngas. Light tars from this method can be removed easily but heavy tars (condensed tertiary products) require extremely high temperatures which result in expensive material cost and lower methane yield.

Catalytic reforming employs catalyst (metal-supported) for converting tars into syngas in a relatively colder environment than thermal decomposition. Cracking is the conversion of only heavy tar molecules into syngas, leaving the light tars unconverted. While reforming reforms all the tars into synthesis gas [41]. Catalytic cracking of tars can occur in-situ or ex-situ of gasifier. The in-situ tar removal is not very effective in transforming all the tars into syngas, so a second reactor is resorted for complete tar removal.

The general reforming reaction of tar is:

$$C_xH_y + x\,H_2O \rightarrow \left(x + \frac{1}{2}y\right)H_2 + CO$$

- Operating temperature & pressure of tar reformer: 900 ºC & 30 bar
- Catalyst used: Biomass Char
- Conversion: 99% [42]

2.7.3.3. Water gas shift:

The optimum ratio for methanation of carbon oxides yields greater quantity of methane and also suppresses the side reactions which results in carbon deposition inside the Methanator. However, the ratio of H_2/CO & H_2/CO_2 in the syngas varies significantly. The reported ratio of H_2/CO & H_2/CO_2 is between (0.8-2.3) and (2.8-3.5). To convert this ratio into optimum required, water-gas shift reactor is positioned before the methanation which increased the ratio of H_2/CO to 3 and H_2/CO_2 to 4. The reaction occurring inside the water-gas shift is:

$$CO + H_2O \rightarrow CO_2 + H_2, \quad \Delta H^0r = -41\,KJ/mol$$

In this process, sour shift is followed (which presumes that catalyst is sulfur tolerant) because carbonyl sulfide compounds are also converted into H_2S in water gas shift reactor. This will allow the subsequent downstream H_2S removal process to get rid all the sulfur (including organic sulfur) which is poisonous for methanation catalyst.

- Operating temperature & pressure: 350ºC & 5 bar.
- Catalyst used: Ni-Al-Cu
- Conversion: 92% [43]

2.7.3.4. Sulfur & carbon dioxide removal:

Almost all of the sulfur in the solid waste is converted into H_2S during gasification which causes chemical deactivation of methanation catalyst. The deactivation results in loss of catalyst activity and life so its elimination becomes necessary for smoother operation in methanation. Both H_2S and excess CO_2 is removed in flour process, where propylene glycol acts as a solvent. This process usually needs lesser energy for regeneration than its competitive amine-based processes because they form chemical bonds with the absorbed gas.

2.7.4. Synthetic natural gas production:

The purified synthesis gas after absorption unit is directed towards methanation section where carbon oxides are hydrogenated to methane and water. Methanation can be understood as a formation of methane from carbon and hydrogen under high pressure and low temperatures due to its thermodynamic favorability at such conditions. Due to sensitive catalyst and high heat of reaction, methanation becomes a challenging problem for process optimization. Following reactions occur in the methanation section,

$$CO + 3\,H_2 \rightleftharpoons CH_4 + H_2O, \quad \Delta H^0r = -206\,KJ/mol$$

$$CO_2 + 4H_2 \rightleftharpoons CH_4 + 2H_2, \quad \Delta H^0r = -165\,KJ/mol$$

$$2CO \rightarrow C + CO_2, \quad \Delta H^0r = -171\,KJ/mol$$

$$CO + H_2 \rightarrow C + H_2O, \quad \Delta H^0r = -131\,KJ/mol$$

Synthesizing methane from CO methanation gained industrial importance during the oil crisis in 1970's. However, due to growing distress of environmental pollution and greenhouse gas emissions, work on CO methanation was resuscitated in 21st century resulting in several technologies that are currently available for CO methanation,

Table 2.6: *CO-Methanation technologies*

CO Methanation Technologies	
Technology Name	**Concept**
Lurgi	Employs 2 FBR's with intermediate cooling and recycling
TREMP	Employs 3-4 FBR's with intermediate cooling and gas recycling
VESTA	Similar to TREMP with and exception of steam addition and no gas recycling.
HICOM	Employs 3 FBR's with intermediate cooling and gas recycling
Linde isothermal reactor	Employs 1 isothermal fixed bed reactor

Temperature profile inside the methanation reactor is used to distinguish between different methanation technologies while seminove number is used for differentiating between different methanation reactors by heating and cooling rate.

Table 2.7: *Seminove number of reactors*

Reactor Type	Temperature Profile	Seminove Number
Fixed Bed	Adiabatic, Isothermal and Polytropic	∞, 0, $0 < Se\# > \infty$
Fluidized Bed	Isothermal	0

Despite of high seminove number and adiabatic temperature profile, fixed bed methanation is preferred due to its high reaction kinetics and better opportunities of heat integration. While in fluidized bed, mechanical abrasion of particles with reactor walls will result in catalyst loss thus requiring makeup catalyst along with the need of cleaning the product gas from abraded material. Difference between methanation reactors is given below,

Table 2.8: *Methanation reactors*

	Fixed Bed	Fluidized Bed
Particle Size	**millimeters**	**micrometers**
Mechanical Stress	Low	High
Thermal Stress	High	Low
Heat Integration	High	Low

2.7.4.1. Catalyst selection:

Group 8-10 catalyst are usually considered for methanation process due to their greater activity and selectivity towards methane. The order proposed by Mills et al. for selectivity of catalyst towards methane is [44],

Selectivity: Ni > Co > Fe > Ru
Activity: Ru > Fe > Ni > Co > Mo

- Ruthenium, having the greatest activity but low selectivity, forms higher hydrocarbons in methanation reaction. Moreover, it is 120 times more expensive than nickel.
- Same is the case of iron which have low selectivity towards methane.
- Nickel is the most employed methanation catalyst due to its higher selectivity, durability at extreme temperatures and relatively lesser cost.
- Cobalt is almost comparable to nickel but is relatively expensive.
- Molybdenum have lowest activity towards methanation but it has high tolerability to sulfur poisoning.

2.7.4.2. Catalyst supports & promoters:

Metal oxides such as alumina, silica or titania are used as catalysts support in order to,

- Enlarge catalyst active surface area.
- Increase catalyst activity.

Out of three mentioned above, alumina with gamma modification is most commonly used because of its high specific surface area, large average pore diameter and more uniform distribution of active component [45]. Occasionally promoters such as MgO are also used that enhances thermal stability of the catalyst and also prevents the formation of fouling by carbon deposits. But these promoters are usually avoided because they may increase the selectivity towards higher hydrocarbons.

2.7.4.3. Catalyst deactivation:

During methanation, catalyst may undergo several deactivations [46]:

- Thermal Deactivation.
- Chemical Deactivation.
- Mechanical Deactivation.

2.7.4.3.1. Thermal deactivation:

This type of deactivation occurs due to extreme temperatures inside the reactor which results in local hotspots and sintering. Sintering causes a decrease in catalyst activity and loss of active surface area. However, such high temperatures can be endured by nickel catalyst without having any significant effect on its selectivity.

2.7.4.3.2. Chemical deactivation:

Chemical deactivation of methanation catalyst may result due to sulfur poisoning of nickel catalyst or vapor-solid reactions. Vapor-solid reactions occurs at temperature of 200 ºC, where carbon monoxide reacts with nickel to form nickel-tetracarbonyls. But such temperatures are usually avoided because of lower activity of nickel catalyst below 230 ºC. However, vapor solid reactions may also occur due to reaction of carbon monoxide with iron. So, heat exchangers whose construction material is iron should be replaced by stainless steel or other suitable material.

2.7.4.3.3. Mechanical deactivation:

Mechanical deactivation is due to abrasion of catalyst particles with reactor walls or other particles that results from pressure fluctuations inside the reactor. Also, variable synthesis gas flowrate may be one of the causes of catalyst stressing. However, these problems are limited to only fluidized bed reactors.

- Operating temperature & pressure: 350-750 ºC & 5 bar.
- Conversion: 98% [47]
- Process Selection: TREMP

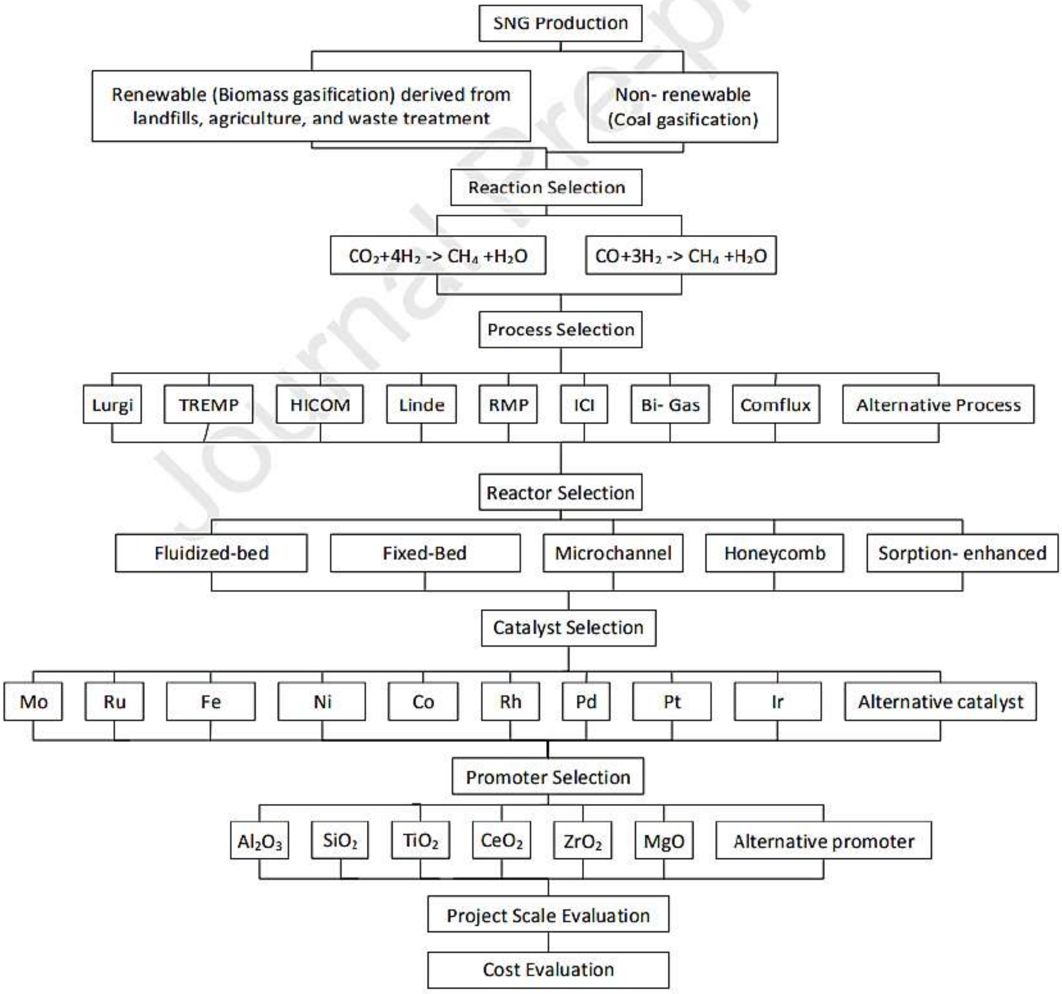


***Figure 2.9:** Road map for SNG production by methanation (source: Google Scholar)*

- Reactor Selection: **Fixed Bed**
- Catalyst Selection: **Ni based**
- Promoter Selection: **γ-Al_2O_3**

2.7.5. Gas conditioning:

The gas from the methanation is then sent to the conditioning section where excess moisture is removed and wobbe index is adjusted, to commensurate fossil natural gas, by injecting propane or nitrogen.

2.8. Capacity selection:

Requirement of solid waste for production of proposed SNG plant = 1000 tons/day.
(Gothenburg biomass gasification plant capacity = 660 tons/day) [48]
Total amount of solid waste generated in Lahore = 5000 tons/day
Waste collected by LWMC = 2500 tons/day

CHAPTER # 03

MATERIAL BALANCE

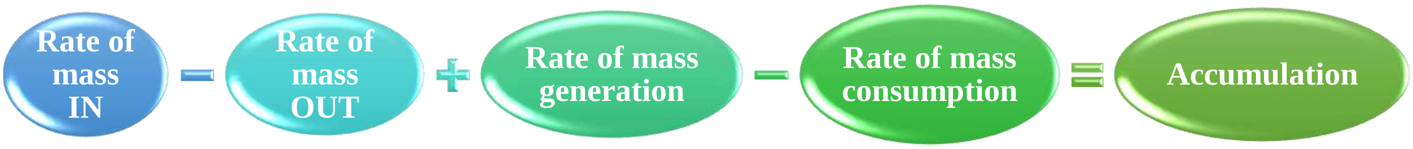
3. Material balance:

Mass balance or material balance is an application of the law of conservation of mass that states that mass can neither be created nor destroyed. The accounting of mass into and out of the system is necessary in order to determine the flowrates of each species involve in the process. The confirmation of flowrates of each species is necessary to maintain the end product quality, environmental regulations and by-products quantity. The application of law of conservation of mass can be applied by different mass balance techniques namely,

- Compound balance.
- Elemental species balance.
- Extent of reaction.

The design of all unit operations and processes are set by mass balances whereby the flowrates of streams are used to setup relationship between different streams. Also, mathematical modelling of chemical or physical processes into analytical equations is done through mass balances.

3.1. General material balance equation:



Assumptions:

- Steady state

Basis:

- 1 hr of operation

Capacity[1]**:**

- 1000 tons per day.

$$= \frac{\mathbf{1000\ tons * 1000\ kg * 1\ day}}{\mathbf{day * 1\ ton * 24\ hr}} = \mathbf{41666} \frac{\mathbf{kg}}{\mathbf{hr}}$$

3.1.1. Material balance on dryer:

Table 3.1: *Proximate and ultimate analysis of solid waste*

Proximate analysis of solid waste (percent)	
Moisture	51.87
Volatile matter	27.44
Fixed carbon	5.87
Ash	14.82

Ultimate analysis of solid waste (percent)	
Carbon	55.2
Hydrogen	2.72
Oxygen	38.53
Nitrogen	1.95
Sulfur	1.6

---

[1] Basis: per 1 hr. of operation

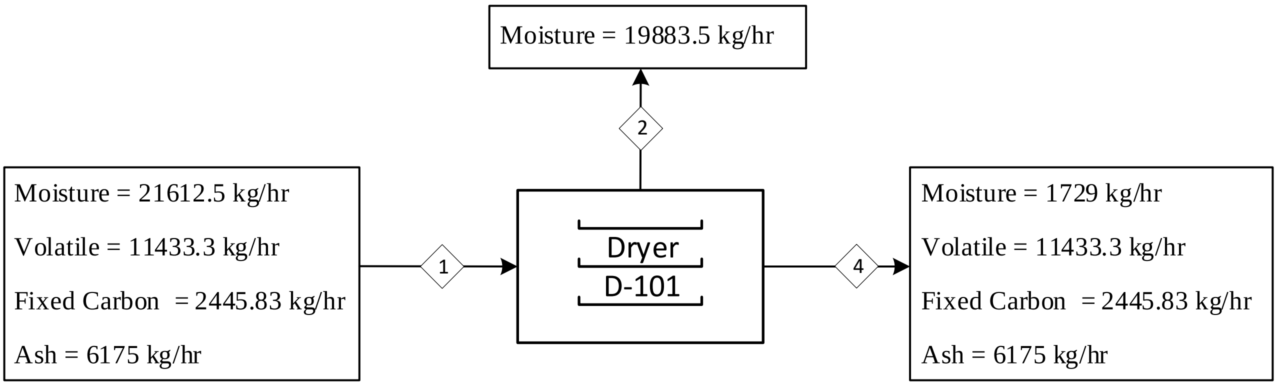


Figure 3.1: *Balance on dryer (D-101)*

As reported from literature that dryer efficiency is 92% [49]. So, flowrates of the streams are,

Table 3.2: *Mass balance on dryer*

Flowrates (kg/hr.)			
Stream no.	**1**	**2**	**4**
Title	**Solid Waste Feed**	**Moisture**	**Dried Solid Waste**
Component	**Inlet**	**Outlet**	
Moisture	21612.5	19883.5	1729
Volatile	11433.3	-	11433.3
Fixed Carbon	2445.83	-	2445.83
Ash	6175	-	6175
Total	**41666**	**41666**	

3.1.2. Material balance on torrefaction[2] unit:

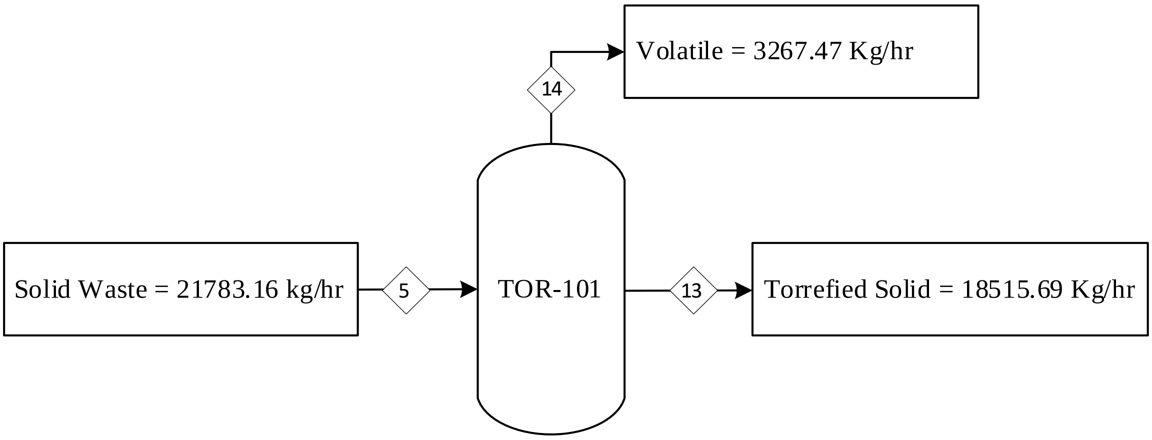


Figure 3.2: *Balance on torrefaction unit*

From the reported literature, it is found that volatiles yield in torrefaction is up to 15% of the solid waste and rest goes to yield torrefied solid.

Table 3.3: *Material balance on torrefaction unit*

Flows (kg/hr.)			
Steam no.	**5**	**14**	**13**
Title	**Dried solid waste**	**Volatiles**	**Torrefied Solid**
Component	**Inlet**	**Outlet**	
Solid Waste	21783.16	-	18515.69
Volatiles	-	3267.47	-
Total	**21783.16**	**21783.16**	

Volatiles from the torrefaction unit consists only CO and CO_2. So molar flowrate of volatiles can be found by,

$$Volatiles = \left(\frac{3267.475}{MW^{3}} + \frac{3267.475}{MW^{4}}\right) \tag{3.1}$$

$$= 190.9 \frac{kmol}{hr.}$$

- Percentage of carbon monoxide in volatiles = 30 %
- Percentage of carbon dioxide in volatiles = 70 %

---

[2] Nitrogen is fed to create an inert environment and will not be continuously fed or withdrawn from the torrefaction unit.

[3] Molecular weight of CO

[4] Molecular Weight of CO2

3.1.3. Material balance on gasification unit:

The individual component flowrates in the torrefied solid waste is found through ultimate analysis.

Table 3.4: *Ultimate analysis*

Component	Mass flowrates (kg/hr.)	Molar flowrates (kmol/hr.)
Carbon	10220.66	850.94
Hydrogen	503.63	249.81
Oxygen	7134.10	222.94
Nitrogen	361.06	12.89
Sulfur	259.22	8.08

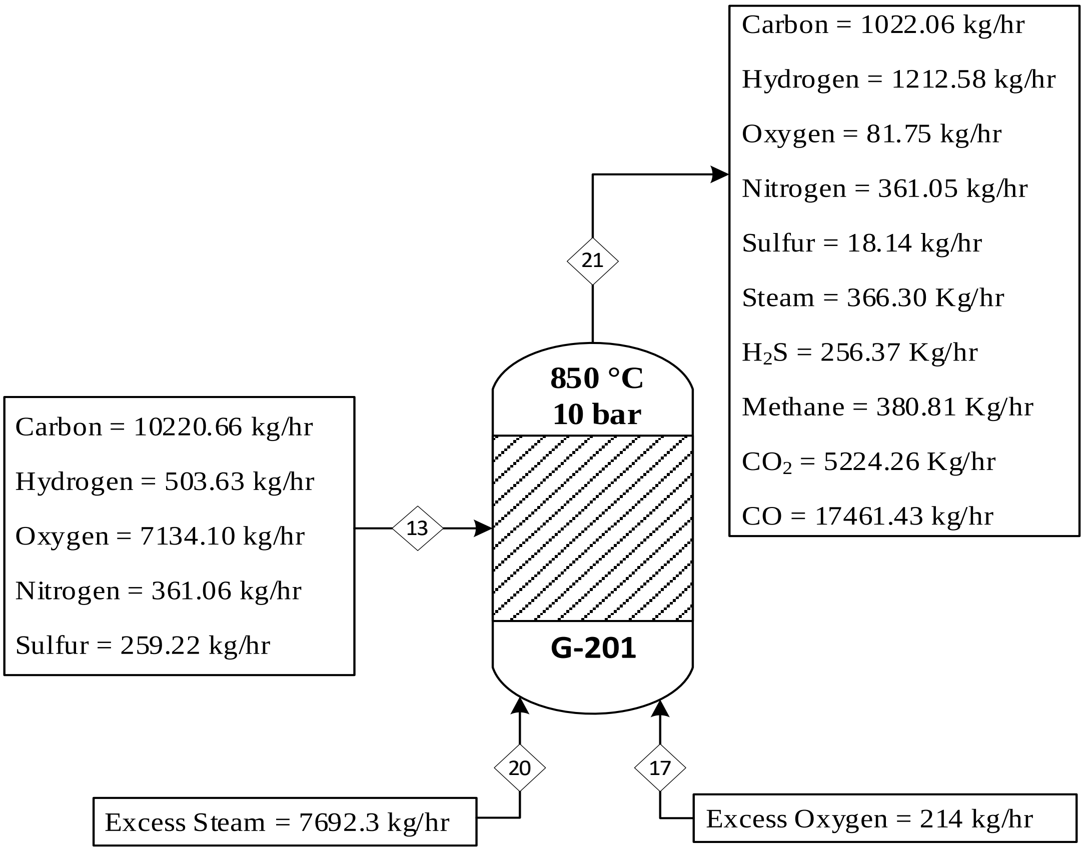


Figure 3.3: *Balance on gasifier unit*

Reactions occurring in the gasification reactor are.

$$C(s) + H_2O(v) \rightarrow CO(g) + H_2(g) \ldots\ldots\ldots\ldots X_a = 0.531[5] \tag{3.2}$$

$$C(s) + O_2(g) \rightarrow CO_2(g) \ldots\ldots\ldots\ldots X_a = 0.155 \tag{3.3}$$

$$C(s) + 2H_2(g) \rightarrow CH_4(g) \ldots\ldots\ldots\ldots X_a = 0.031 \tag{3.4}$$

$$S(s) + H_2(g) \rightarrow H_2S(g) \ldots\ldots\ldots\ldots X_a[6] = 0.93 \tag{3.5}$$

$$C(s) + \frac{1}{2} O_2(g) \rightarrow CO(g) \ldots\ldots\ldots\ldots X_a = 0.283 \tag{3.6}$$

---

[5] Reference for conversion of gasification reactions is given in detailed process description discussed in chapter 2.

[6] Conversion of Sulfur

The total carbon conversion is 90%. So, the carbon available to take part in reaction is 9198.59 kg/hr. or 765.84 kmol/hr. The carbon conversion distributed among several reactions is listed above. It should be observed that carbon conversion in the above reactions reach 100 % because the carbon that is available for reaction is reacted completely.

For reaction (01)	
Carbon conversion	**0.531**
Reacted carbon	406.66
CO produced	406.66
H_2 produced	406.66
H_2O required	406.66

For reaction (02)	
Carbon conversion	**0.155**
Reacted carbon	118.706
CO_2 produced	118.706
O_2 required	118.706

For reaction (03)	
Carbon conversion	**0.031**
Reacted carbon	23.741
CH_4 produced	23.741
H_2 required	47.48

For reaction (04)	
Sulfur conversion	**0.93**
Reacted Sulfur	7.51
H_2S produced	7.51
H_2 required	7.51

For reaction (05)	
Carbon conversion	**0.283**
Reacted carbon	216.73
CO produced	216.73
H_2 required	108.367

- Oxygen intrinsically in the feed = 222.94 kmol/hr.
- Oxygen required for reaction = 227.07 kmol/hr.

So, excess air should be provided to fulfill stoichiometric amount of oxygen. Let the excess air fed to gasifier is 3%.

- **Excess air fed = 31.84 kmol/hr**. (The amount of excess air should be calculated based on the difference between actual air (convert O_2 in feed to air)[7] and air in which excess amount is added i.e., 1.03*Air fed. So,
- **Oxygen in excess air = 6.68 kmol/hr.**

Now, the stoichiometric amount of steam required for reactions is 406.6 kmol/hr. Let the excess steam fed is 5%. So, total steam fed to gasifier is 426.99 kmol/hr.

Table 3.5: *Mass balance on gasification unit*

Stream no.	**7**		**8**		**9**		**10**	
Stream	**Torrefied solid**		**Excess oxygen**		**Excess Steam**		**Syngas**	
Component	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**
Carbon	10220.66	850.94	-	-	-	-	1022.06	85.1
Hydrogen	503.63	249.81	-	-	-	-	1212.58	601.47
Oxygen	7134.10	222.94	214	6.68	-	-	81.75	2.55
Nitrogen	361.06	12.89	-	-	-	-	361.05	12.89
Sulfur	259.22	8.08	-	-	-	-	18.14	0.56
Steam	-	-	-	-	7692.3	426.99	366.30	20.33
Hydrogen sulfide	-	-	-	-	-	-	256.37	7.51
Methane	-	-	-	-	-	-	380.81	23.74
Carbon dioxide	-	-	-	-	-	-	5224.26	118.70
Carbon monoxide	-	-	-	-	-	-	17461.43	623.39
Total (kg/hr.)	**26385**						**26385**	

- **Composition of tar in syngas:**
  - As syngas from gasifier contains tars such as naphthalene, styrene, xylene, indene, biphenyl, dibenzofuran, fluorene, anthracene, pyrene and fluoranthene.
  - We are only considering naphthalene as a modal component in tar because of its highest percentage. From the literature [50], it is reported that syngas contains 0.42% of tars and tars contain 40 % of naphthalene. So, naphthalene in synthesis gas is,

Naphthalene in syngas = 0.42*26385 ⟹ 44.32 kg/hr.

Now subtracting mass of naphthalene from syngas. Syngas tar free is 26340 kg/hr. As the tars from the syngas is subtracted the mass of the individual component is disturbed. So, normalizing technique should be applied for mass conservation. Percentage or mole fraction of components in syngas containing tars,

Table 3.6: *Mole fraction of syngas composition*

---

[7] 1 kmol air = 0.21 kmol O_2

Component	**Mol fraction**[8]
Carbon	0.056
Hydrogen	0.401
Oxygen	0.0017
Nitrogen	0.0086
Sulfur	0.0003
Steam	0.0135
Hydrogen sulfide	0.0050
Methane	0.0158
Carbon dioxide	0.0793
Carbon monoxide	0.4166
Sum	**1**

Molar flowrate of syngas (tar free)[9] = 1495.9 kmol/hr
Now, molar flowrates of components in syngas having no tars,

Table 3.7: *Molar flowrate of component*

Component	**Molar flowrate**[10] **(kmol/hr.)**
Carbon	85.07
Hydrogen	601.34
Oxygen	2.55
Nitrogen	12.89
Sulfur	0.56
Steam	20.32
Hydrogen sulfide	7.51
Methane	23.73
Carbon dioxide	118.67
Carbon monoxide	623.25
Syngas tar free	1495.94
Naphthalene	0.345

Here we have separated naphthalene as a separate entity from syngas.

---

[8] Individual component moles/Total moles of outlet stream
[9] Syngas molar flowrate – Naphthalene flowrate
[10] Molar flowrate of syngas (tar free) *Mole fraction

3.1.4. Material balance on mixing point:

Table 3.8: *Mass balance on mixing point.*

Stream no.	**21**		**14**		**22**	
Stream	**Syngas from Gasifier**		**Volatiles from Torrefaction unit**		**Syngas**	
Component	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**
C	1021.82	85.07	-	-	1021.83	85.07
H_2	1212.30	601.34	-	-	1212.30	601.34
O_2	81.73	2.55	-	-	81.74	2.55
N_2	360.97	12.89	-	-	360.97	12.89
S	18.14	0.56	-	-	18.14	0.56
Steam	366.21	20.32	-	-	366.22	20.32
H_2S	256.31	7.51	-	-	256.31	7.51
CH_4	380.72	23.73	-	-	380.72	23.73
CO_2	5223.06	118.67	5882.27	133.65	11105.33	252.3
CO	17457.39	623.25	1604.46	57.28	19061.86	680.5
$C_{10}H_8$	44.32	0.34	-	-	44.32	0.34
Sum (kg/hr.)	**33909.76**				**33909.76**	

3.1.5. Material balance on cyclone separator:

- Efficiency of cyclone separator = 100 %

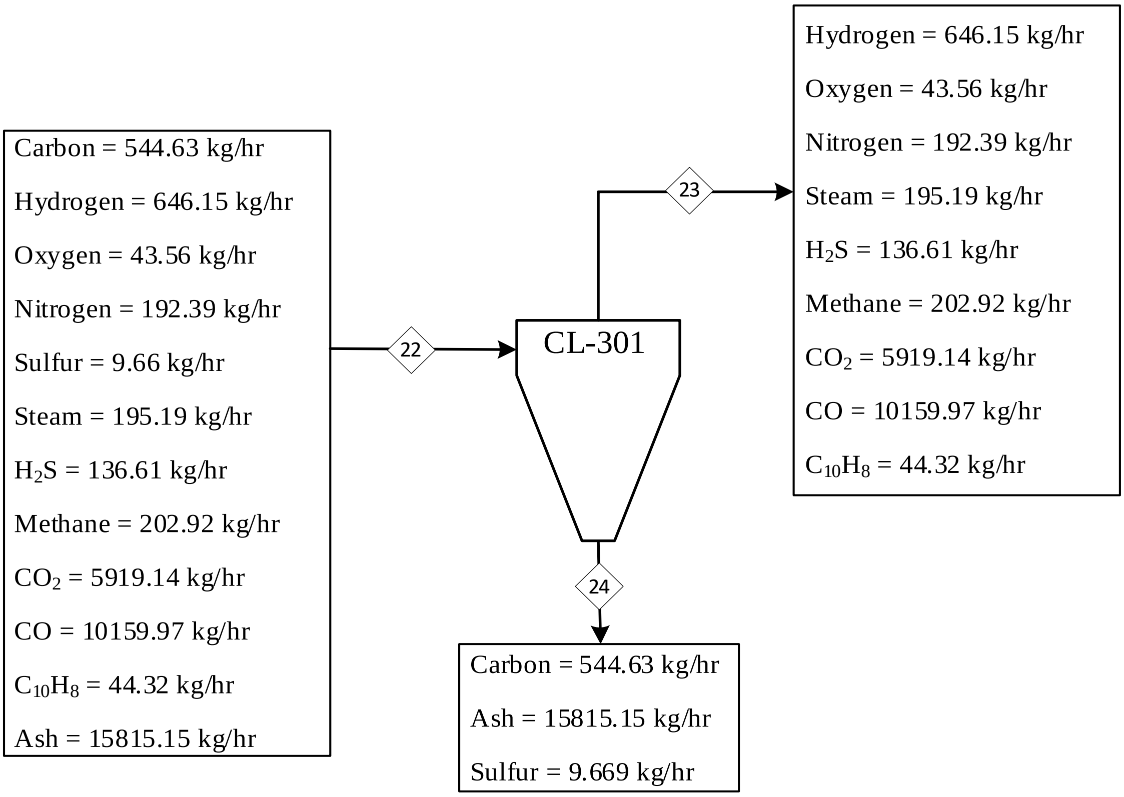


***Figure 3.4:** Balance on cyclone separator unit*

Cyclone separator will separate the solid particles and ash formed in the gasification section. Now, separating ash from the syngas as a separate entity.

***Table 3.9:** Equivalent weight percent*

Stream no.	**22**	
Component	**Mass flow (kg/hr.)**	**Wt. (%)**
C	1021.82	0.030
H_2	1212.30	0.035
O_2	81.73	0.0024
N_2	360.97	0.010
S	18.14	0.0005
Steam	366.21	0.010
H_2S	256.31	0.007
CH_4	380.72	0.011
CO_2	11105.33	0.32
CO	19061.86	0.56
Syngas	33865.43	1
$C_{10}H_8$	44.32	1

- From the gasification reactor, ash is also formed which is about 46.7% of the synthesis gas. So, mass flowrate of ash is 15815.15 kg/hr. Now as the flowrate of total syngas is disturbed so individual components flowrates are again found via normalization technique. The mass flowrate of syngas without ash is 18050.2 kg/hr.

Table 3.10: *Mass balance on cyclone separator unit*

Flows (kg/hr.)			
Stream no.	**22**[11]	**24**	**23**
Stream	**Syngas containing ash**	**Ash**	**Clean Syngas**
Component	**Mass flowrate**	**Mass flowrate**	**Mass flowrate**
C	544.63	544.63	-
H_2	646.15	-	646.15
O_2	43.56	-	43.56
N_2	192.39	-	192.39
S	9.66	9.669	-
Steam	195.19	-	195.19
H_2S	136.61	-	136.61
CH_4	202.92	-	202.92
CO_2	5919.14	-	5919.14
CO	10159.97	-	10159.97
$C_{10}H_8$	44.32	-	44.32
Ash	15815.15	15815.15	-
Total	**33909.75**	**33909.75**	

---

[11] Mass flowrates are found via normalization technique.

3.1.6. Material balance on tar reformer:

$$C_{10}H_8(g) + 10\,H_2O(v) \rightarrow 10\,CO(g) + 14\,H_2(g) \ldots\ldots\ldots X_{a1} = 99.9\%^{12} \qquad (3.7)$$

$$CH_4(g) + H_2O(g) \rightarrow CO(g) + 3\,H_2(g) \ldots\ldots.\ldots.X_{a2} = 60\% \qquad (3.8)$$

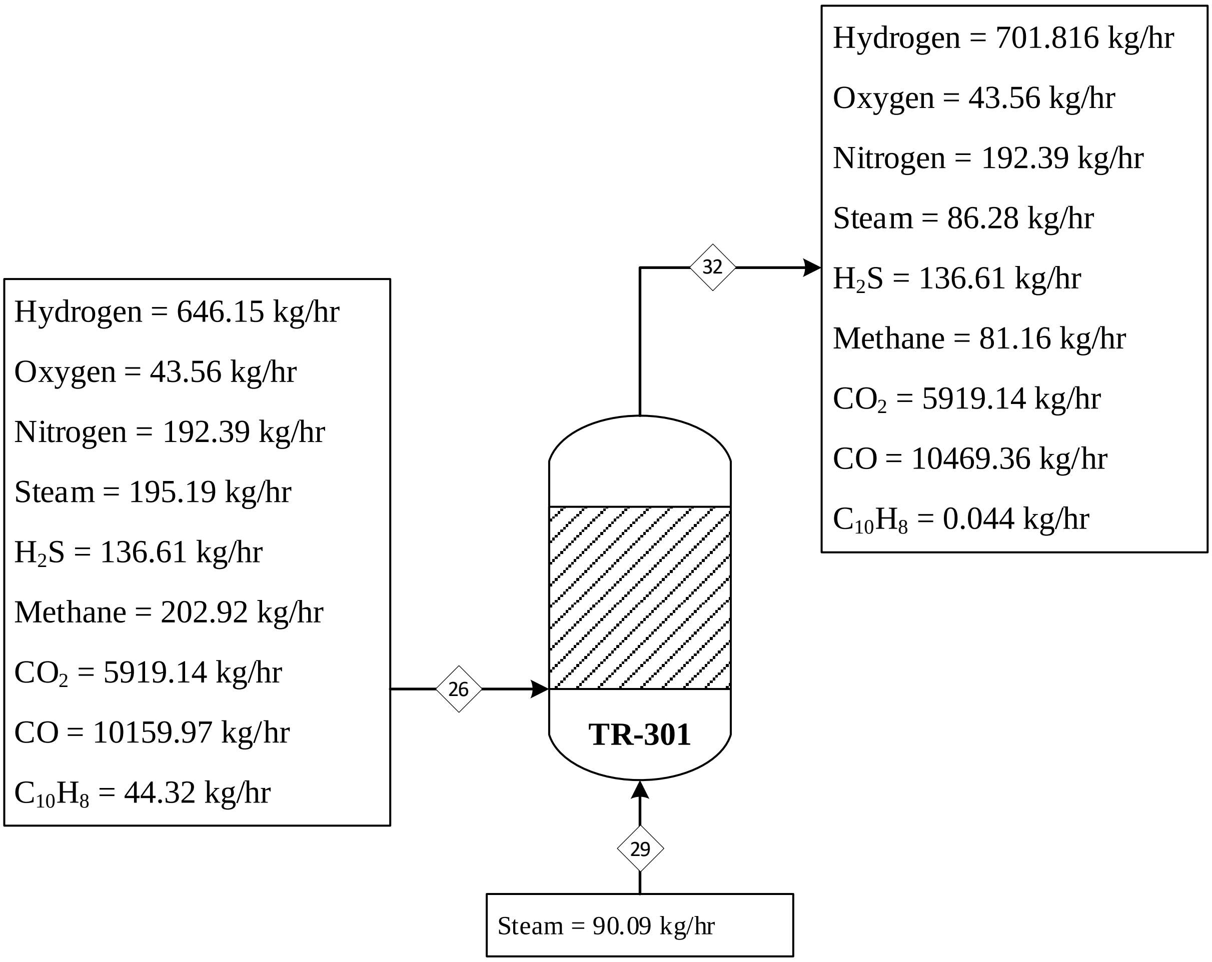


Figure 3.5: *Balance on tar reformer unit*

For reaction (01):	
$C_{10}H_8$ fed	0.345
CO produced	3.454
H_2O required	3.454
H_2 Produced	4.836

For reaction (02):	
CH_4 fed	12.651
CO produced	7.590
H_2O required	7.590
H_2 Produced	22.772

---

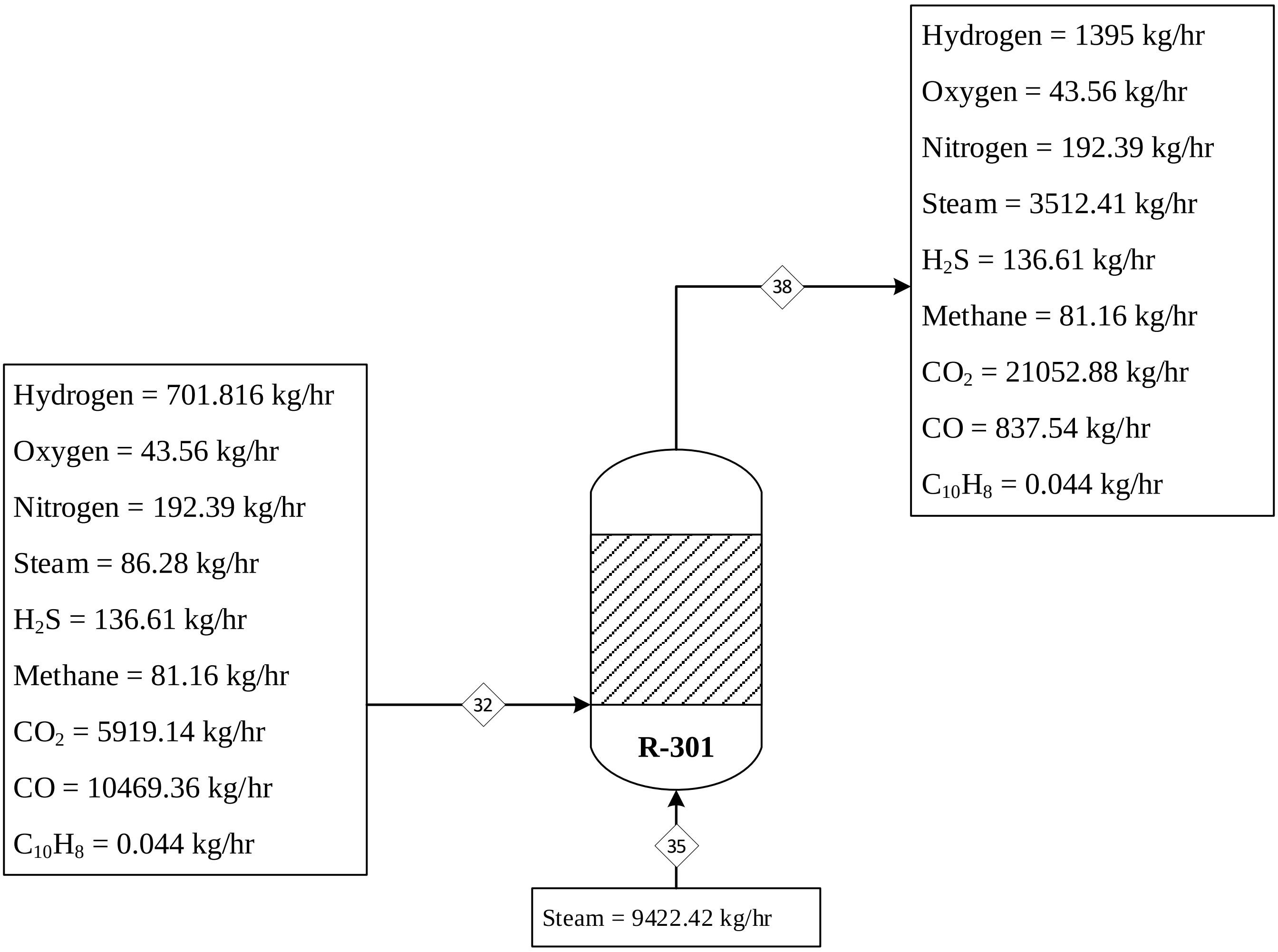
[12] Reference is cited in detailed process description

Table 3.11: *Mass balance on tar reformer*

Stream no.	**26**		**32**	
Stream	**Syngas containing tar**		**Product syngas from tar reformer**	
Component	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**
H_2	646.15	320.51	701.816	348.12
O_2	43.56	1.36	43.56	1.36
N_2	192.39	6.87	192.39	6.87
Steam	285.28	15.83	86.28	4.78
H_2S	136.61	4	136.61	4
CH_4	202.92	12.65	81.16	5
CO_2	5919.14	134.49	5919.14	134.49
CO	10159.97	362.72	10469.36	373.77
$C_{10}H_8$	44.32	0.34	0.044	0.0003
Sum (kg/hr.)	**17630.38**		**17630.38**	

3.1.7. Material Balance on water gas shift reactor:

$$CO(g) + H_2O\,(g) \leftrightarrow CO_2\,(g) + H_2(g) \dots\dots..Xa = 0.92 \qquad (3.9)$$



Hydrogen = 701.816 kg/hr
Oxygen = 43.56 kg/hr
Nitrogen = 192.39 kg/hr
Steam = 86.28 kg/hr
H_2S = 136.61 kg/hr
Methane = 81.16 kg/hr
CO_2 = 5919.14 kg/hr
CO = 10469.36 kg/hr
$C_{10}H_8$ = 0.044 kg/hr

Steam = 9422.42 kg/hr

Hydrogen = 1395 kg/hr
Oxygen = 43.56 kg/hr
Nitrogen = 192.39 kg/hr
Steam = 3512.41 kg/hr
H_2S = 136.61 kg/hr
Methane = 81.16 kg/hr
CO_2 = 21052.88 kg/hr
CO = 837.54 kg/hr
$C_{10}H_8$ = 0.044 kg/hr

Figure 3.6: *Balance on WGS unit*

Table 3.12: *Stoichiometric calculation on WGS*

Stoichiometric calculations	
CO fed	373.77
H_2 produced	343.87
H_2O required	343.87
CO_2 produced	343.87

As stoichiometric requirement of steam exceeds the amount present in the feed so steam must be provided for reaction to occur.

- Amount of steam required for reaction to occur: 343.87 – 4.78 = 339.08 kmol/hr.
- Let the excess steam provided is 57.5 %. Then the steam provided[13] from external source is 534 kmol/hr.

Table 3.13: *Mass balance on water gas shift reactor (WGS)*

---

[13] 339.02*1.575 = 533.9 kmol/hr.

Stream no.	**32**		**38**	
Stream	**Feed to WGS reactor**		**Product stream from WGS reactor**	
Component	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**	**Mass flow (kg/hr.)**	**Molar flow (kmol/hr.)**
H_2	701.81	348.12	1395	691.99
O_2	43.56	1.36	43.56	1.36
N_2	192.39	6.87	192.39	6.87
Steam	9707.7	538.77	3512.41	194.97
H_2S	136.61	4	136.61	4
CH_4	81.16	5.06	81.16	5.06
CO_2	5919.14	134.49	21052.88	478.36
CO	10469.36	373.74	837.54	29.90
$C_{10}H_8$	0.044	0.0034	0.044	0.00034
Total (kg/hr.)	**27251**		**27251**	

3.1.8. Material balance on absorber (01):

- Solubility of CO_2 in Propylene Carbonate (PC) = 120 $\frac{ft3}{gallon}$ [51]
- Solubility of CO_2 in PC = 1.68 $\frac{kg}{lt}$

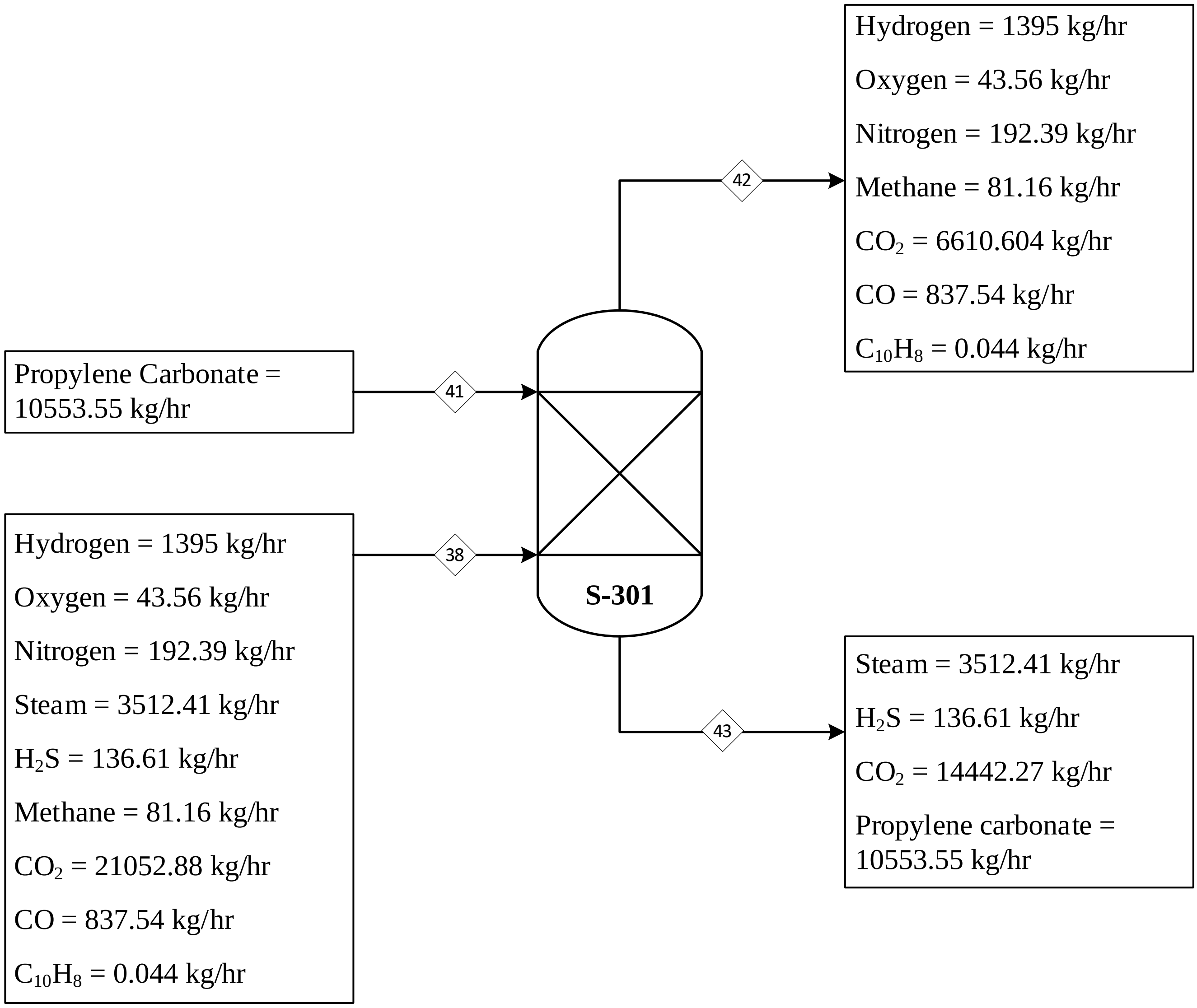


Figure 3.7: *Balance on scrubber (S-301)*

Here we must absorb a fixed percentage of CO_2 in solvent to maintain the methanation ratio (given below) to 3. This ratio is accepted globally in methanation to avoid side reactions, carbon deposition on methanation catalyst and for maximum yield of methane.

$$\frac{H_2 - CO_2}{CO + CO_2} = 3$$

So, solvent required to absorb 68.6%[14] of CO_2 is,

$$= \frac{(0.686 * 21052.88)}{1.68} \rightarrow 8587.74\ \frac{lt}{hr} \qquad (3.10)$$

- Similarly, H_2S solubility in PC = 2.03 $\frac{kg}{lt}$

Quantity of solvent required to absorb all amount of H_2S,

$$= \frac{(136.61)}{2.03} \rightarrow 67.019\ \frac{lt}{hr} \qquad (3.11)$$

---

[14] Percentage that is determined through calculations to keep the desired methanation ratio.

Density of solvent = 1.195 $\frac{kg}{lt}$

So, amount of solvent fed to absorb H_2S and CO_2 = 10342.44 $\frac{kg}{hr}$

Makeup solvent = 2.4 %

- **Total amount of solvent fed = 10553.55** $\frac{kg}{hr}$

From the literature it is also reviewed that at this much amount of solvent, all of the water vapors present gets absorbed in propylene carbonate. So,

Table 3.14: *Mass balance on scrubber (S-301)*

Flows (kg/hr.)				
Stream no.	**38**	**41**	**42**	**43**
Stream	**Inlet**		**Outlet**	
Component	**Feed**	**Lean solvent**	**Tail gases**	**Rich solvent**
H_2	1395.05	-	1395.05	-
O_2	43.56	-	43.56	-
N_2	192.39	-	192.39	-
Steam	3512.41	-	-	3512.41
H_2S	136.61	-	-	136.61
CH_4	81.16	-	81.16	-
CO_2	21052.88	-	6610.604	14442.27
CO	837.54	-	837.54	-
$C_{10}H_8$	0.044	-	0.044	-
$C_4H_6O_3$	-	10553.55	-	10553.55
Total	**37805.25**		**37805.25**	

3.1.9. Material balance on stripper (st-301):

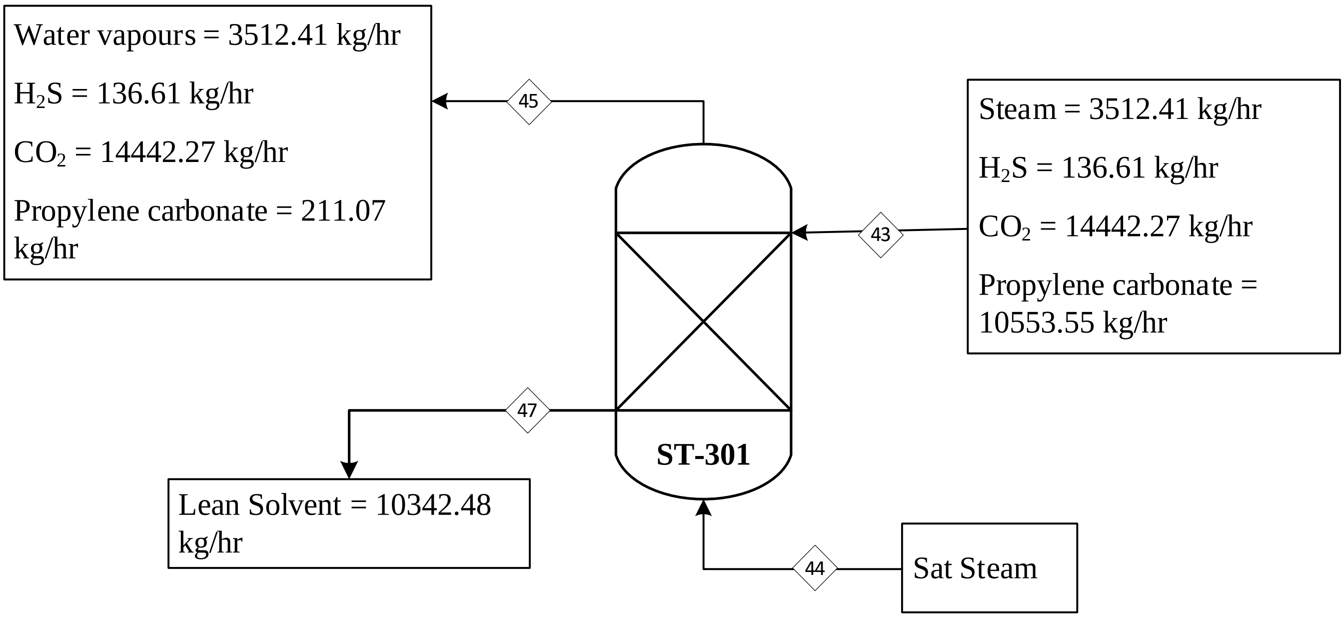


Figure 3.8: *Balance on stripper (ST-301)*

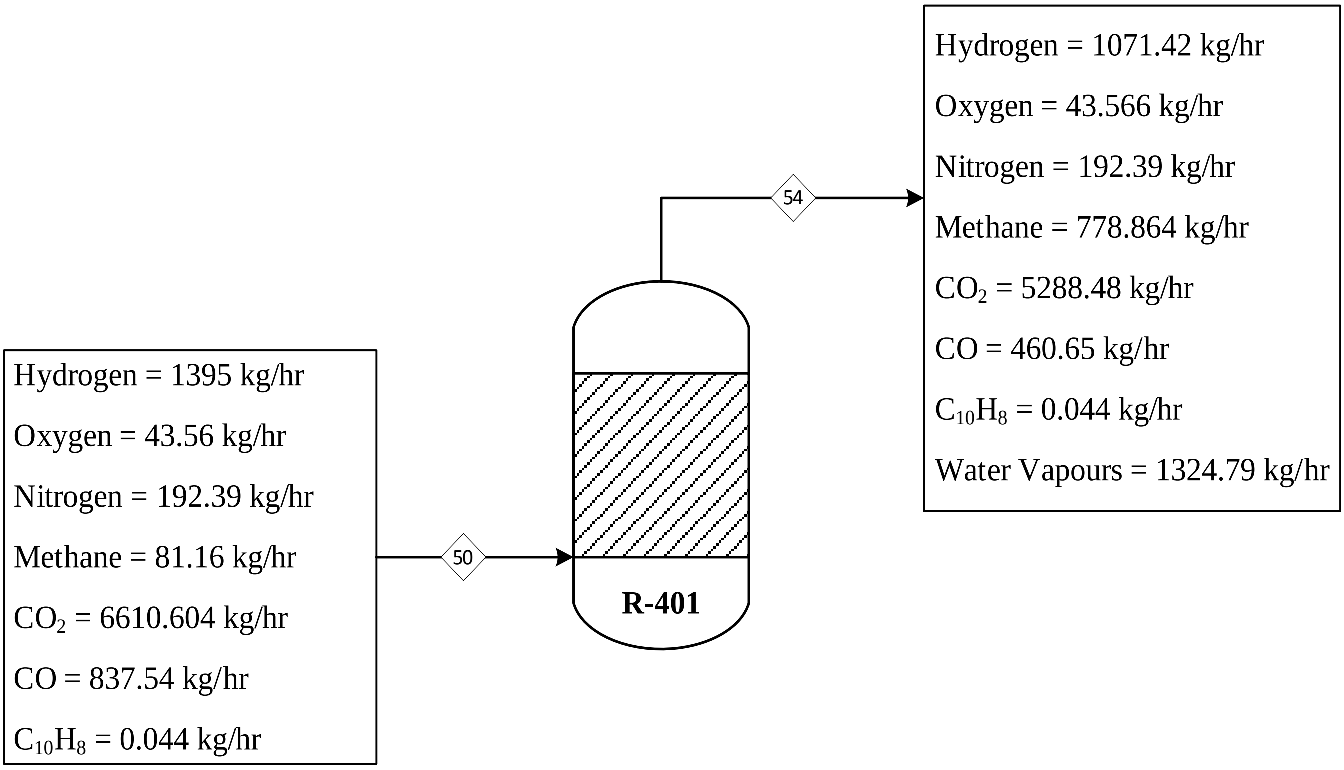
- Solvent lost in the stripper = 2%

Table 3.15: *Material balance on stripper-01*

Flows (kg/hr.)				
Stream no.	**43**	**41**	**47**	**45**
Stream	**Inlet**		**Outlet**	
Component	**Rich solvent**	**Sat. steam**	**Lean solvent**	**Stripped gases**
Water vapors	3512.41		-	3512.41
H_2S	136.61	-	-	136.61
CO_2	14442.27	-	-	14442.27
$C_4H_6O_3$	10553.55	-	10342.48	211.07
Sum	**28644.85**		**28644.85**	

3.1.10. Material balance on methanator (01):

$$Methanation\ ratio = \frac{H_2 - CO_2}{CO + CO_2} = 3$$



Hydrogen = 1071.42 kg/hr
Oxygen = 43.566 kg/hr
Nitrogen = 192.39 kg/hr
Methane = 778.864 kg/hr
CO_2 = 5288.48 kg/hr
CO = 460.65 kg/hr
$C_{10}H_8$ = 0.044 kg/hr
Water Vapours = 1324.79 kg/hr

Hydrogen = 1395 kg/hr
Oxygen = 43.56 kg/hr
Nitrogen = 192.39 kg/hr
Methane = 81.16 kg/hr
CO_2 = 6610.604 kg/hr
CO = 837.54 kg/hr
$C_{10}H_8$ = 0.044 kg/hr

Figure 3.9: *Balance on methanator (R-401)*

$$CO\ (g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(v) \ \ldots\ldots\ldots X_{a1} = 0.45 \tag{3.12}$$

$$CO_2\ (g) + 4H_2(g) \rightarrow CH_4(g) + 2H_2O(v) \ \ldots\ldots\ldots X_{a2} = 0.20 \tag{3.13}$$

Flows (kmol/hr.)	
For reaction (01)	
CO fed	29.90
CH_4 Produced	13.45
H_2 Required	40.36
H_2O Produced	13.45

For reaction (02)	
CO_2 fed	150.20
CH_4 Produced	30.04
H_2 Required	120.16
H_2O Produced	60.08

Table 3.16: *Mass balance on methanator-1*

Flows (kmol/hr.)				
Stream no.	**50**		**54**	
Stream	**Inlet**		**Outlet**	
Component	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**
H_2	1395.09	691.99	1071.42	531.46
O_2	43.566	1.36	43.566	1.36
N_2	192.39	6.87	192.39	6.87
CH_4	81.16	5.06	778.864	48.55
CO_2	6610.6	150.20	5288.48	120.16
CO	837.54	29.91	460.65	16.44
$C_{10}H_8$	0.044	0.00034	0.044	0.00034
Water vapors	-	-	1324.79	73.538
Sum (kg/hr.)	**9160**		**9160**	

3.1.11. Material balance on methanator (02):

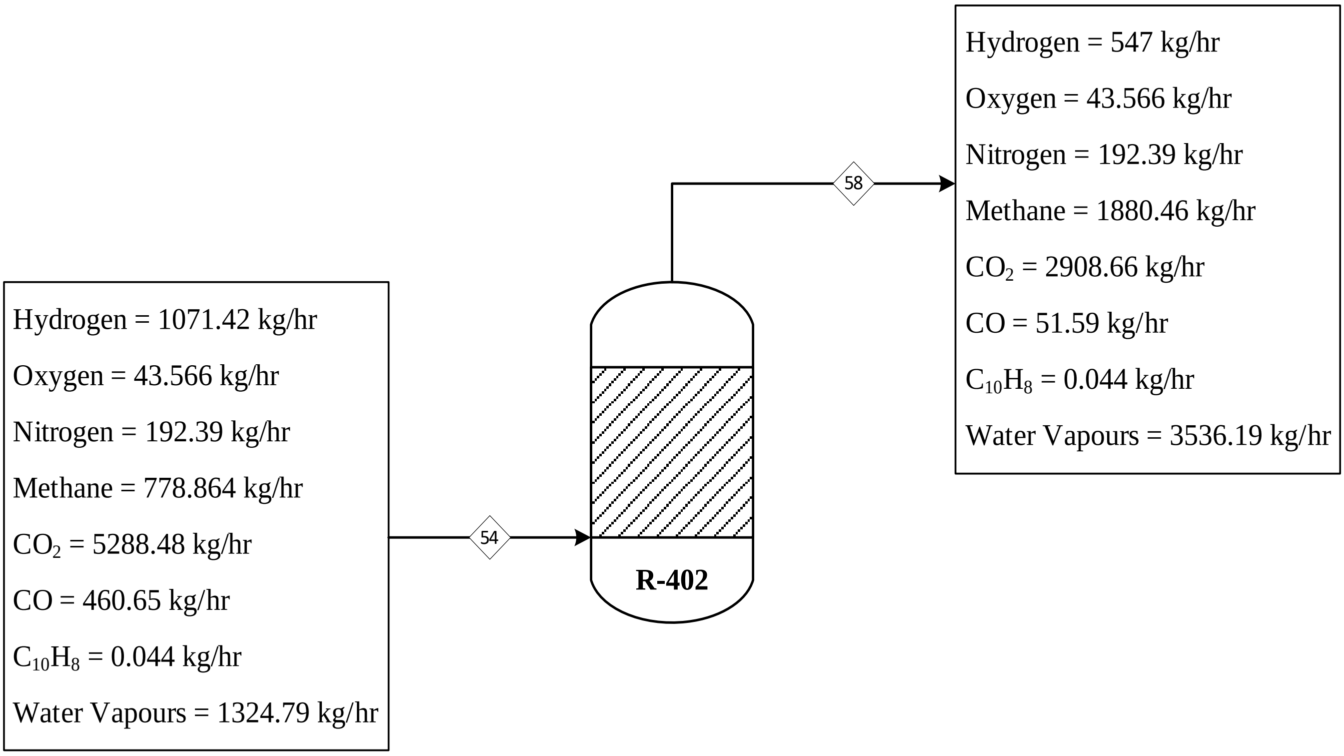


Figure 3.10: *Balance on methanator (R-402)*

$$CO\ (g)\ +\ 3\ H_2(g)\ \rightarrow\ CH_4(g)\ +\ H_2O(v)\ \ldots\ldots\ldots X_{a1}\ =\ 0.888 \tag{3.14}$$

$$CO_2\ (g) +\ 4\ H_2(g) \rightarrow\ CH_4(g) +\ 2\ H_2O(v)\ \ldots\ldots\ldots X_{a2}\ =\ 0.45 \tag{3.15}$$

Flows (kmol/hr.)	
For reaction (01)	
CO fed	16.44
CH_4 Produced	14.60
H_2 Required	43.81
H_2O Produced	14.60

For reaction (02)	
CO_2 fed	120.16
CH_4 Produced	54.07
H_2 Required	216.29
H_2O Produced	108.14

Table 3.17: *Mass balance on methanator-2*

Flows (kmol/hr.)				
Stream no.	**54**		**58**	
Stream	**Inlet**		**Outlet**	
Component	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**
H_2	1071.42	531.46	547	271.35
O_2	43.566	1.36	43.566	1.36
N_2	192.39	6.87	192.39	6.87
CH_4	778.8	48.55	1880.46	117.23
CO_2	5288.48	120.16	2908.66	66.09
CO	460.65	16.44	51.59	1.84
$C_{10}H_8$	0.044	0.00034	0.044	0.00034
Water vapors	1324.79	73.53	3536.19	196.29
Sum (kg/hr.)	**9160**		**9160**	

3.1.12. Material balance on methanator (03):

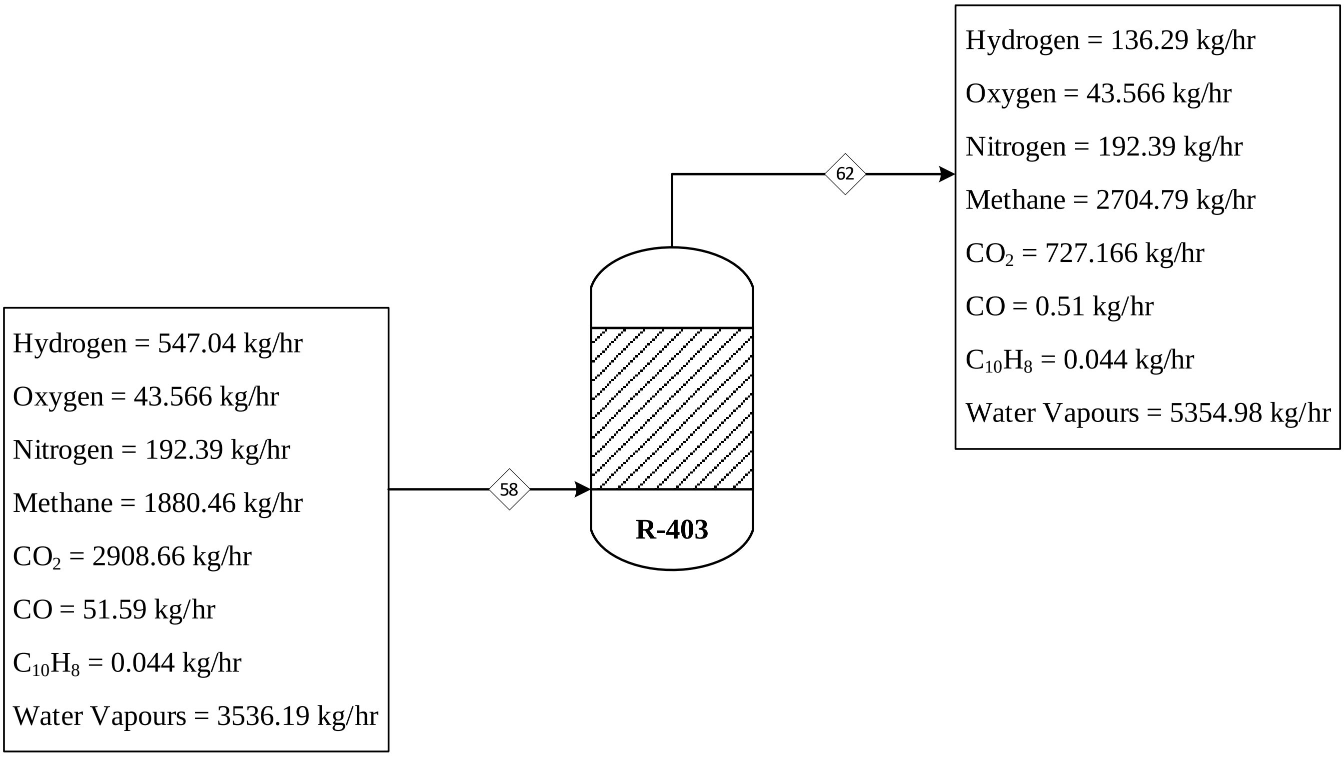


Figure 3.11: *Balance on methanator (R-403)*

$$CO\ (g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(v) \ \ldots\ldots\ldots X_{a1} = 0.99 \tag{3.16}$$

$$CO_2\ (g) + 4\,H_2(g) \rightarrow CH_4(g) + 2H_2O(v) \ \ldots\ldots\ldots X_{a2} = 0.75 \tag{3.17}$$

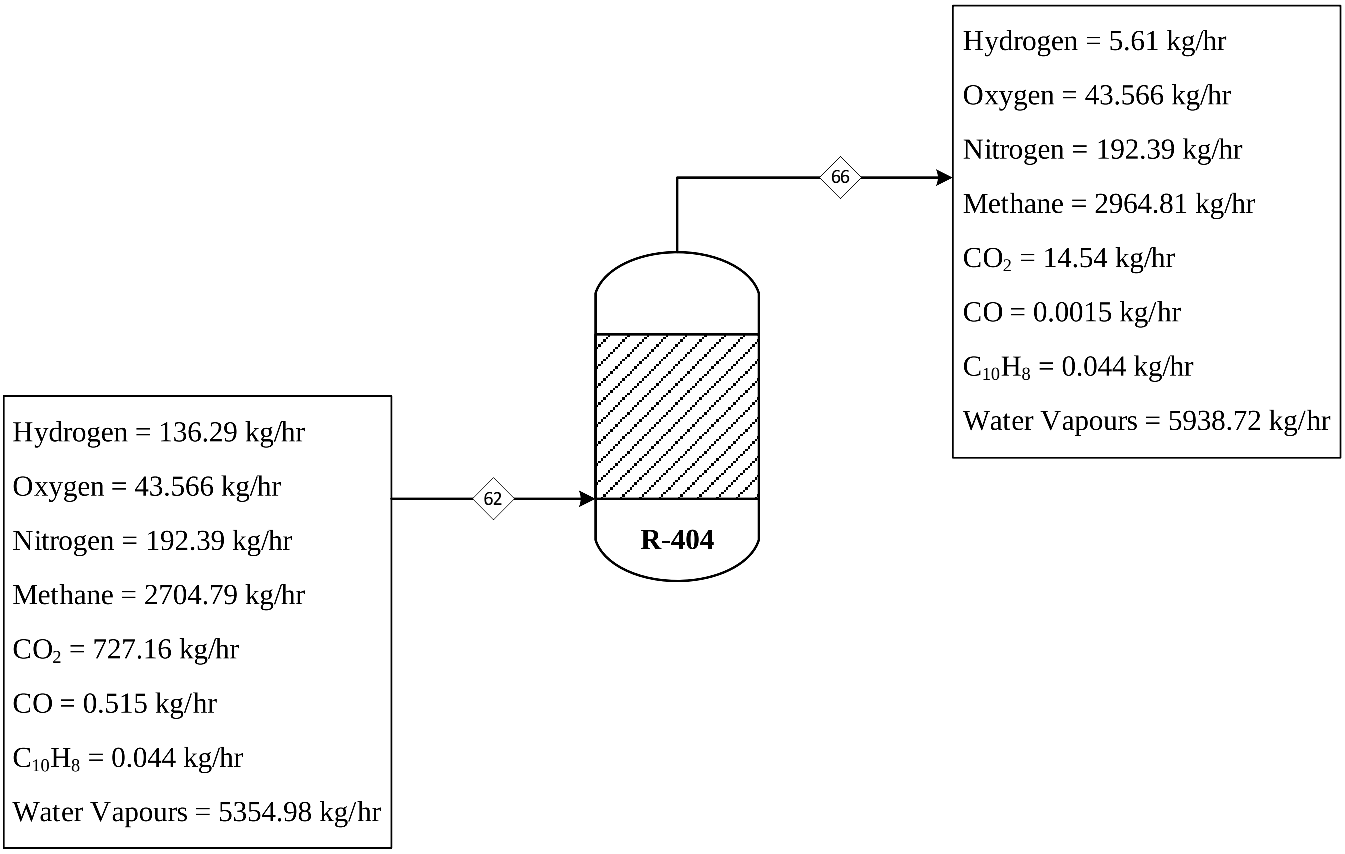
For reaction (01)	
CO fed	1.84
CH_4 Produced	1.82
H_2 Required	5.47
H_2O Produced	1.82

For reaction (02)	
CO_2 fed	66.09
CH_4 Produced	49.56
H_2 Required	192.27
H_2O Produced	99.13

Table 3.18: *Mass balance on methanator -3*

Flows (kmol/hr)				
Stream no.	**58**		**62**	
Stream	**Inlet**		**Outlet**	
Component	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**
H_2	547.04	271.35	136.29	67.60
O_2	43.566	1.36	43.566	1.36
N_2	192.39	6.87	192.39	6.87
CH_4	1880.46	117.23	2704.79	168.62
CO_2	2908.66	66.09	727.166	16.52
CO	51.59	1.841	0.51	0.018
$C_{10}H_8$	0.044	0.00034	0.044	0.00034
Water vapors	3536.19	196.29	5354.98	297.25
Sum (kg/hr.)	**9160**		**9160**	

3.1.13. Material Balance on methanator (04):



Hydrogen = 5.61 kg/hr
Oxygen = 43.566 kg/hr
Nitrogen = 192.39 kg/hr
Methane = 2964.81 kg/hr
CO_2 = 14.54 kg/hr
CO = 0.0015 kg/hr
$C_{10}H_8$ = 0.044 kg/hr
Water Vapours = 5938.72 kg/hr

Hydrogen = 136.29 kg/hr
Oxygen = 43.566 kg/hr
Nitrogen = 192.39 kg/hr
Methane = 2704.79 kg/hr
CO_2 = 727.16 kg/hr
CO = 0.515 kg/hr
$C_{10}H_8$ = 0.044 kg/hr
Water Vapours = 5354.98 kg/hr

Figure 3.12: *Balance on methanator (R-404)*

$$CO\ (g) + 3\ H_2(g) \rightarrow CH_4(g) + H_2O(v) \ \ldots\ldots\ldots X_{a1} = 0.997 \tag{3.18}$$

$$CO_2\ (g) + 4\ H_2(g) \rightarrow CH_4(g) + 2\ H_2O(v) \ \ldots\ldots\ldots X_{a2} = 0.98 \tag{3.19}$$

For reaction (01)	
CO fed	0.018
CH_4 Produced	0.018
H_2 Required	0.055
H_2O Produced	0.0183

For reaction (02)	
CO_2 fed	16.52
CH_4 Produced	16.19
H_2 Required	64.76
H_2O Produced	32.38

Table 3.19: *Mass balance on methanator -4*

Stream no.	**62**		**66**	
Stream	**Inlet**		**Outlet**	
Component	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**	**Mass flowrate (kg/hr.)**	**Molar flowrate (kmol/hr.)**
H_2	136.29	67.60	5.61	2.78
O_2	43.566	1.36	43.566	1.36
N_2	192.39	6.87	192.39	6.87
CH_4	2704.79	168.62	2964.81	184.83
CO_2	727.16	16.52	14.54	0.33
CO	0.515	0.018	0.0015	5.52E-05
$C_{10}H_8$	0.044	0.00034	0.044	0.00034
Water vapors	5354.98	297.25	5938.72	329.65
Sum (kg/hr.)	**9160**		**9160**	

3.1.14.Material balance on hydro-cyclone:

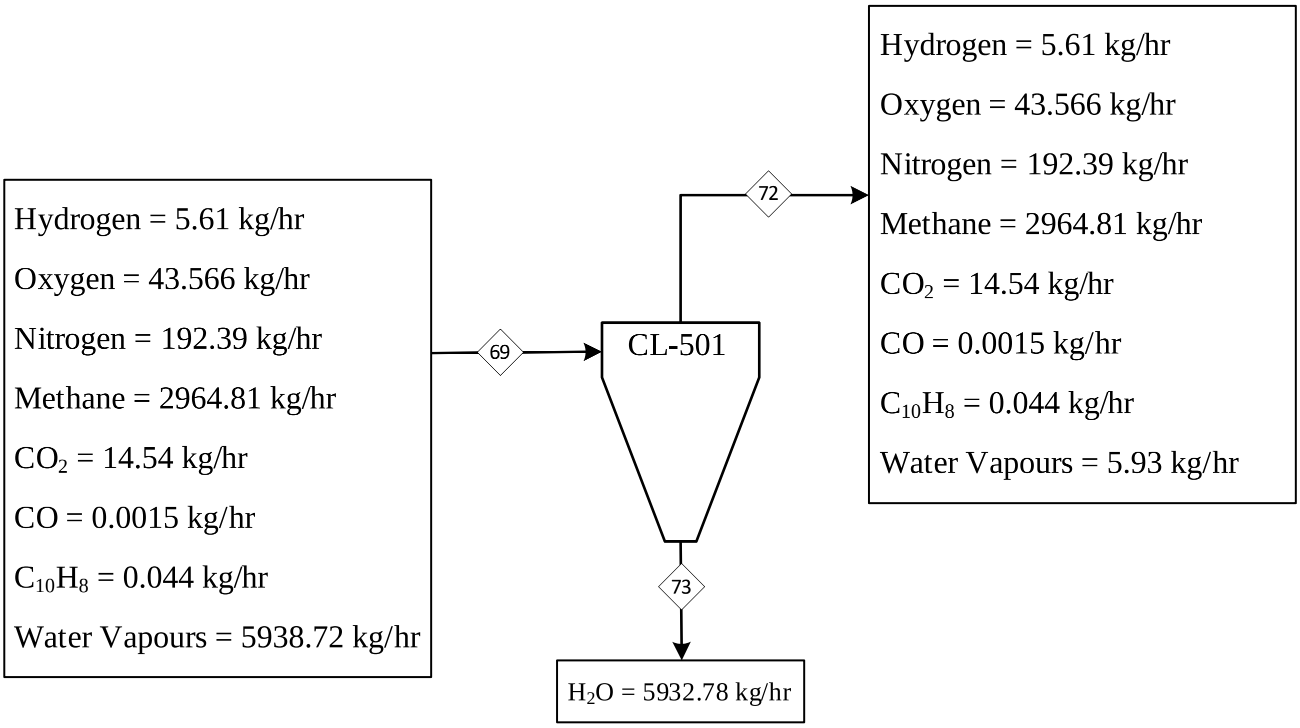


Figure 3.13: *Balance on hydro-cyclone (CL-501)*

- Hydro cyclone efficiency = 99.9%

Table 3.20: *Mass balance on hydro-cyclone*

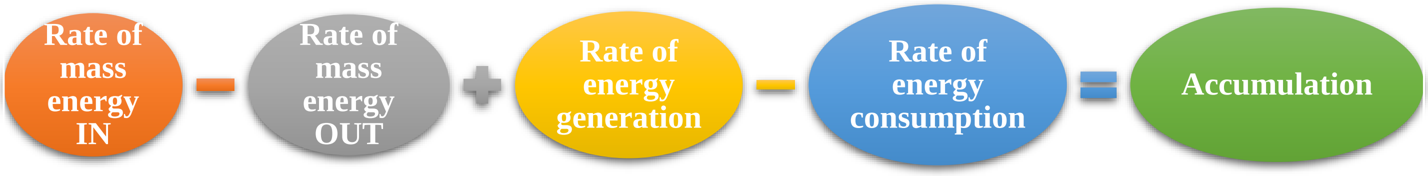
Flows (kg/hr.)			
Stream no.	**69**	**73**	**72**
Stream	**Inlet**	**Outlet**	
Component	**Feed with water**	**Water Content**	**Pure SNG**
H_2	5.61	-	5.61
O_2	43.566	-	43.566
N_2	192.39	-	192.39
H_2O	5938.72	5932.78	5.93
CH_4	2964.81	-	2964.81
CO_2	14.54	-	14.54
CO	0.0015	-	0.0015
$C_{10}H_8$	0.044	-	0.044
Sum	**9160**	**9160**	

CHAPTER # 04

ENERGY BALANCE

4. Energy balance:

The estimates of the energy requirements for the operation, such as heating, cooling, temperature, friction, and enthalpy, are known as energy balance. Kinetic energy, potential energy, heat energy, electrical energy, and mechanical energy are all types of energy. Energy cannot be produced or lost, according to the law of conservation. A general equation of conservation of energy is:



It is also called 1st law of thermodynamics. The total enthalpy of outlet stream is not equal to inlet stream if it's generated or consumed.

Formula used:

$$\hat{H} = \int_{Tref}^{T} Cp * dT \qquad (4.1)$$

$$\hat{H} = a*(T-T_{ref}) + \left(\frac{b}{2}\right)*(T^2-T^2_{ref}) + \left(\frac{c}{3}\right)*(T^3-T^3_{ref}) + \left(\frac{d}{4}\right)*(T^4-T^4_{ref}) \qquad (4.2)$$

4.1. Energy balance on dryer:

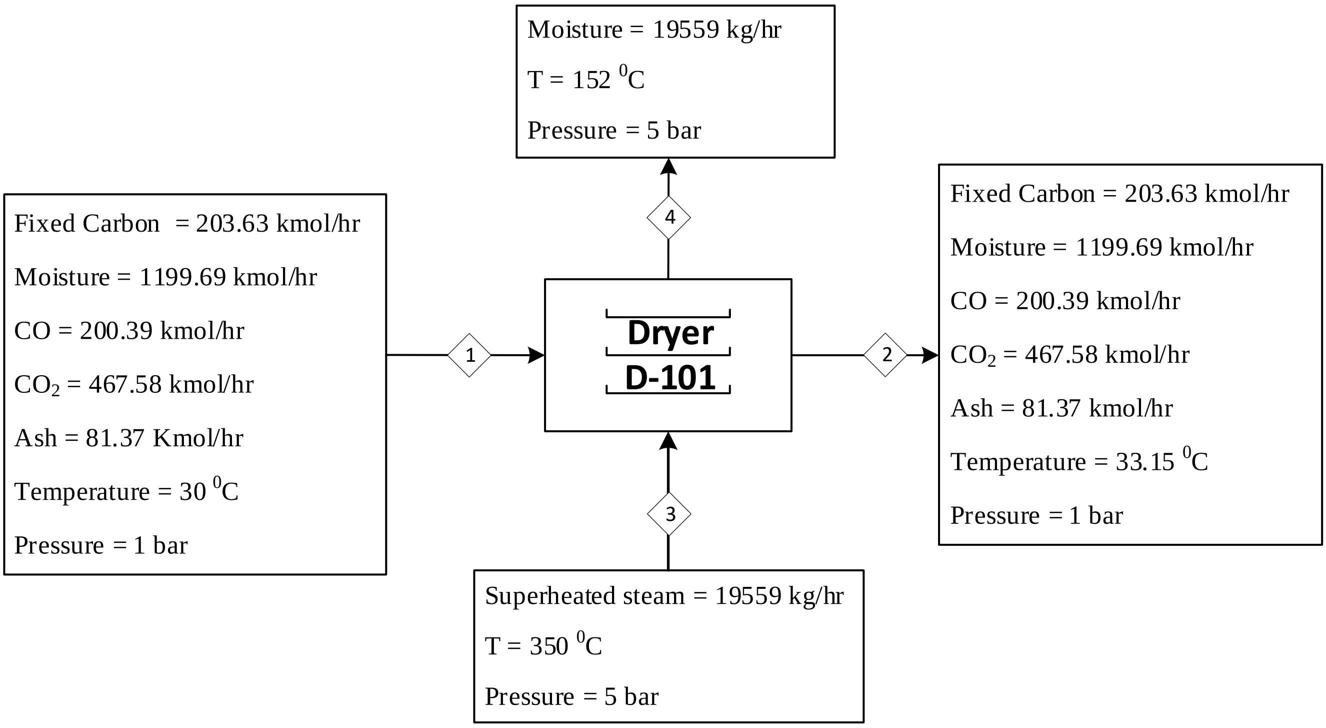


Figure 4.1: *Energy balance on dryer (D-101)*

Table 4.1:*Proximate analysis of solid waste*

Proximate analysis of solid waste[15]	
Fixed carbon	C
Moisture	H_2O
Volatile matter	CO & CO_2
Ash (%) [52]	CaO (0.99) SiO_2 (67.2) Al_2O_3 (24) Fe_2O_3 (5.63) TiO_2 (0.96) Na_2O (0.67) MgO (0.38) K_2O (0.17)

Table 4.2: *Energy balance on dryer*

Stream no.	**1**		**2**	
Stream	**Inlet**			
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
C	203.63	$\widehat{H1}$	203.63	$\widehat{H5}$
H_2O	1199.69	$\widehat{H2}$	1199.69	$\widehat{H6}$
CO	200.39	$\widehat{H3}$	200.39	$\widehat{H7}$
CO_2	467.58		467.58	
Ash	81.37	$\widehat{H4}$	81.37	$\widehat{H8}$
Pressure. bar	1			
Temperature °C	30		33.15	
Reference Temperature °C	25			

- The flowrates of the individual constituents were found via percentage of individual constituent in solid waste (identified through proximate analysis).

---

[15] Based on wet basis

Table 4.3: *Steam condition*

Superheated steam conditions	
Inlet temperature °C	350
Outlet temperature °C	152
Enthalpy at inlet temperature °C	57 kJ/mol.
Enthalpy$_{(liq)}$ at outlet temperature °C	11.54 kJ/mol.
Pressure. bar	5

4.1.1. Inlet and outlet enthalpy:

Enthalpy of inlet streams		
Component	**Enthalpy (kJ/mol.)**	
C	$\widehat{H1}$	97.87
H_2O	$\widehat{H2}$	0.37
CO	$\widehat{H3}$	0.14
CO_2		0.18
Ash	$\widehat{H4}$	0.36

Enthalpy of outlet streams		
Component	**Enthalpy (kJ/mol.)**	
C	$\widehat{H5}$	60.06
H_2O	$\widehat{H6}$	0.61
CO	$\widehat{H7}$	0.23
CO_2		0.304
Ash	$\widehat{H8}$	0.59
Water vapors	$\widehat{H9}$	44.71

- The enthalpy of water vapors was found through = **$(Cp_1 * \Delta T_1 + \lambda + Cp_2 * \Delta T_2)$**[16].
- The outlet temperature of process stream was found via iterative method while conforming to the concept of inlet enthalpies must balance the outlet enthalpies i.e.,

$$H_{in}\ by\ process\ stream + H_{in}\ by\ superheated\ steam = H_{out}\ by\ condensate + H_{out}\ by\ process\ stream \tag{4.3}$$

  - From the above equation H_{out} of the process stream was found and justified with outlet temperature through iterations.

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \tag{4.4}$$

$$(\boldsymbol{\Delta H})^{\cdot} = \mathbf{41346188.3}\ (\boldsymbol{kJ/hr.})$$

---

[16] ΔT_1 refers to temperature change up-to boiling point with respect to reference temperature as T_1 and ΔT_2 refers to temperature change up to steam outlet temperature with respect to boiling point as T_1.

Table 4.4: *Utility requirement for dryer*

Utility Requirement	
$\dot{Q} = m * Cp * \dot{\Delta}\mathrm{T} + \mathrm{m} *\lambda$	
λ at 5 bars	2106.9 kJ/kg
$\dot{m}$	19559 kg/hr.

4.2. Energy balance on torrefaction unit:

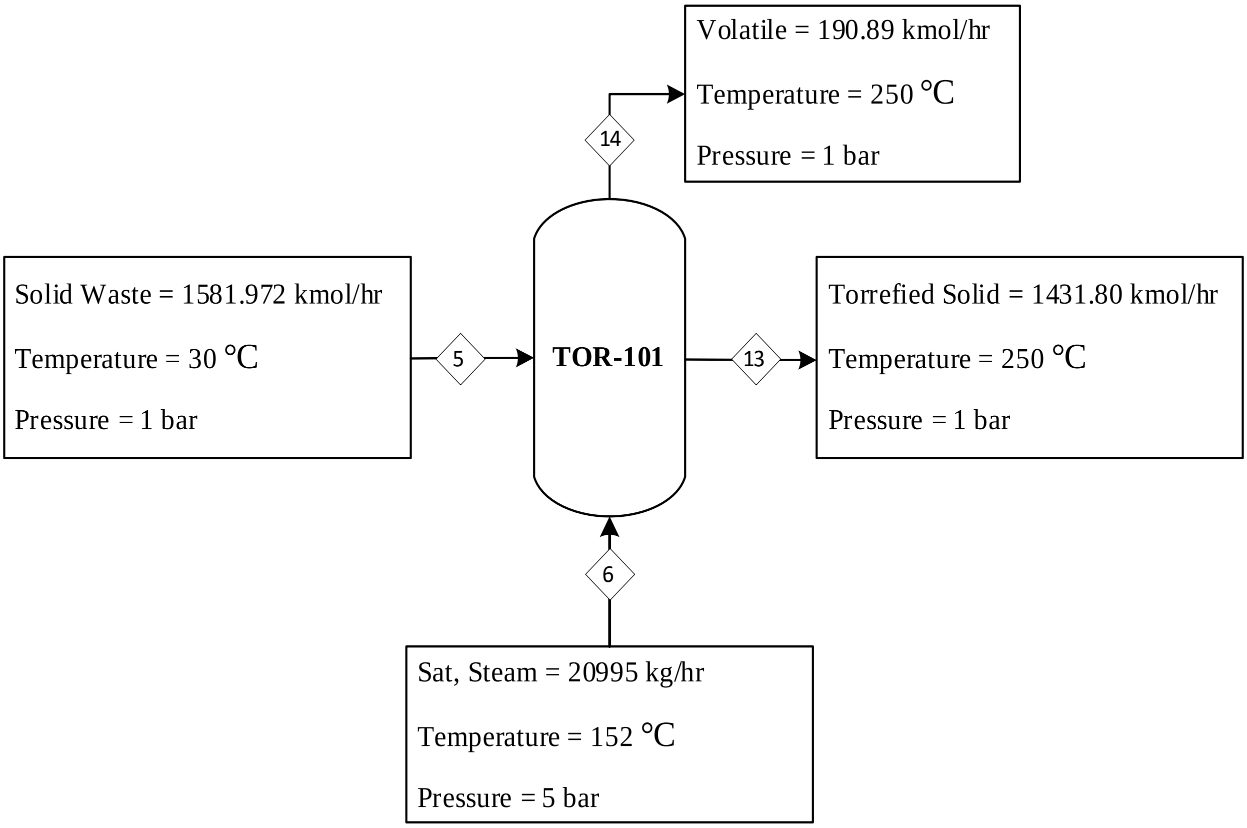


Figure 4.2: *Energy balance on torrefaction unit (TOR-101)*

- Now using enthalpy balance and finding utility requirement of torrefaction unit.

Table 4.5: *Energy balance on torrefaction unit*

Stream no.	**5**		**14, 13**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
Solid Waste	1581.97202	$\widehat{H1}$	-	-
Volatiles (CO & CO_2)	-	-	190.89	$\widehat{H2}$
Torrefied Solid	-	-	1431.80	$\widehat{H3}$
Pressure. Bar	1			
Temperature °C	30		250	
Reference Temperature °C	30			

4.2.1. Inlet and outlet enthalpy for torrefaction unit:

Table 4.6: *Enthalpy of inlet stream would be zero because it is at reference state.*

Enthalpy of outlet streams			
	Component	**Enthalpy (kJ/mol.)**	
Volatiles	Carbon monoxide	$\widehat{\boldsymbol{H}2}$	6.42
	Carbon dioxide		8.98
Solid waste	Carbon	$\widehat{\boldsymbol{H}3}$	5.01
	Hydrogen		6.27
	Oxygen		6.63
	Nitrogen		6.38
	Sulfur		4.53

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \tag{4.5}$$

$$(\boldsymbol{\Delta\ H})^{\cdot} = \mathbf{44234206.31}\ \boldsymbol{kJ/hr}.$$

Table 4.7: *Utility requirement for torrefaction unit.*

Utility Requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \lambda$	
λ at 5 bars	2106.9 kJ/kg
$\dot{\boldsymbol{m}}$	20,995 kg/hr.

4.3. Energy balance on E-201:

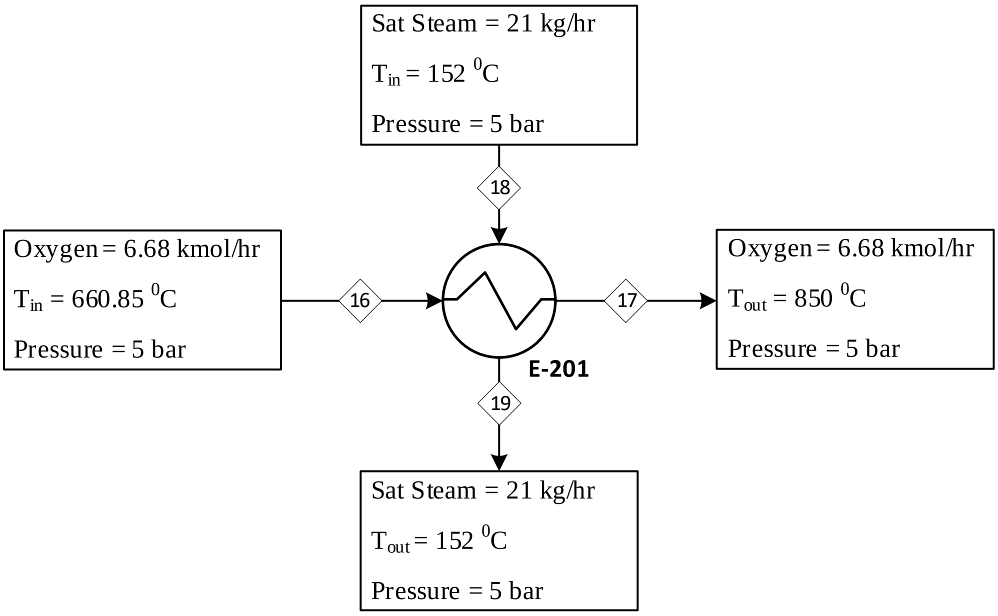


Figure 4.3: *Energy balance on E-201.*

- Now using enthalpy balance and finding utility requirement of heat exchanger unit.

Table 4.8: *Energy balance on E-201.*

Stream no.	**16**		**17**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
Oxygen	6.68	$\widehat{H1}$	6.68	$\widehat{H2}$
Pressure bar	5			
Temperature °C	660.85		850	
Reference Temperature °C	25			

4.3.1. Inlet and outlet enthalpy of E-201:

Table 4.9: *Inlet and outlet enthalpy of E-201.*

Enthalpy of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
Oxygen	$\widehat{H1}$	20.5

Enthalpy of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
Oxygen	$\widehat{H2}$	27.11

It should be observed that pressure of both the inlet and outlet streams is greater than 1 bar. So, correction in heat capacity as a function of pressure must be applied via Edmister's chart.

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \tag{4.6}$$

$$(\boldsymbol{\Delta H})^{\cdot} = \mathbf{44196.45}\ \boldsymbol{kJ/hr}.$$

Table 4.10: *Utility requirement for E-201.*

Utility Requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \lambda$	
λ at 5 bars	2106.9 kJ/kg
$\dot{\boldsymbol{m}}$	21 kg/hr.

4.4. Energy balance on gasifier (G-201):

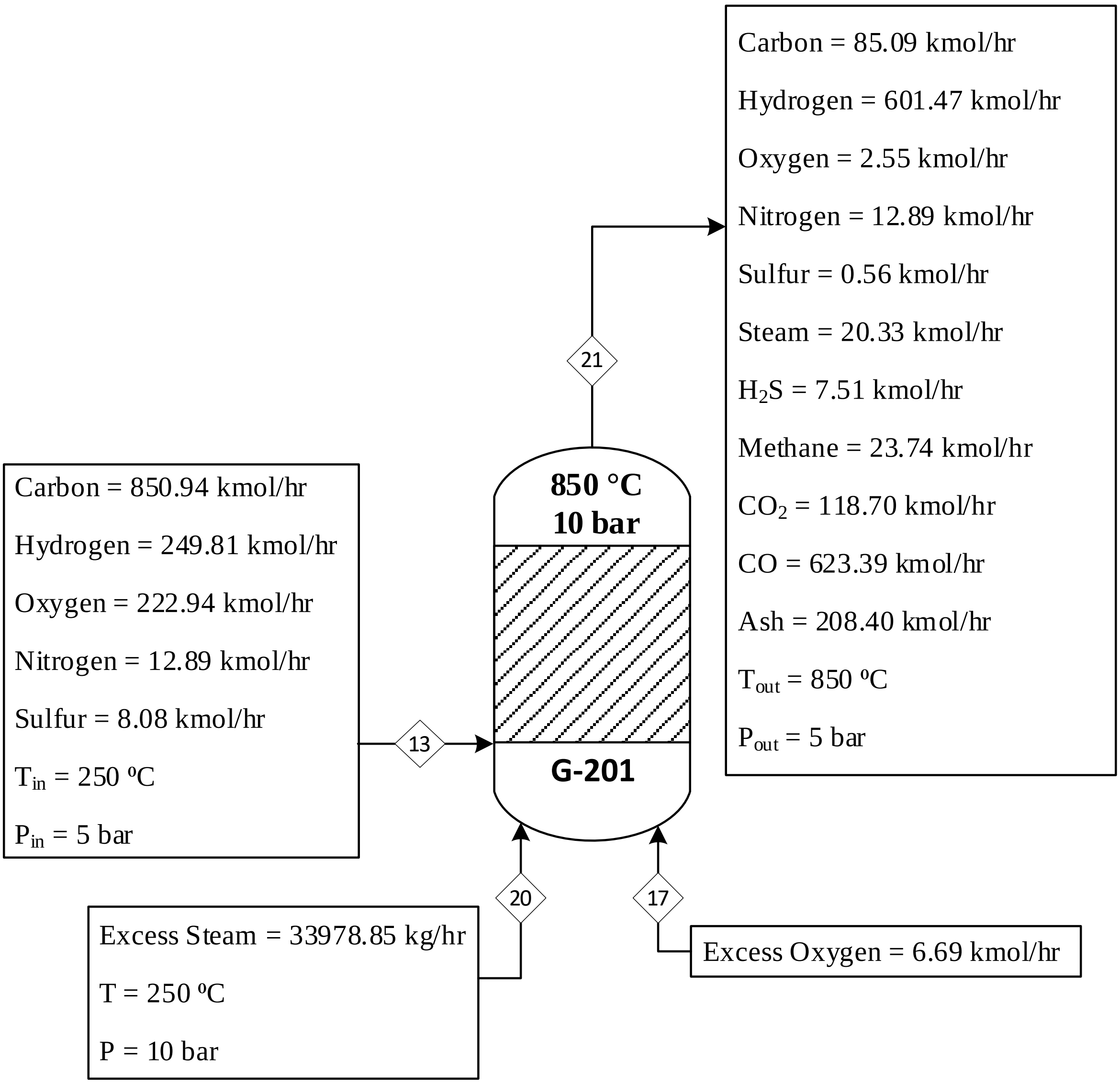


Figure 4.4: *Energy balance on gasifier (G-201)*

Two methods are usually used for performing energy balance around a reactor.

- Heat of formation method and
- Heat of reaction method.

Heat of formation method is usually used when multiple reactions are involved and when heat of reaction is unknown. Heat of formation method is applied here because there is a relative ease in calculation through this method.

In heat of formation method,

$$Specific\ enthalpy\ changes\ or\ \widehat{\boldsymbol{H}} = \boldsymbol{\Delta H} fo + \int_{Tr}^{T} \boldsymbol{a} + \int_{Tr}^{T} \boldsymbol{bT} + \int_{Tr}^{T} \boldsymbol{cT^2} + \int_{Tr}^{T} \boldsymbol{dT^3} \qquad (4.7)$$

Table 4.11: *Heat of formation of components*

Heat of formation of different substances ΔH_f^o	
Components	**ΔH_f^o (kJ/mol.)**
Carbon	0.00
Hydrogen	0.00
Oxygen	0.00
Nitrogen	0.00
Sulfur	0.00
Steam	-241.83
Hydrogen Sulfide	-19.96
Methane	-74.85
Carbon dioxide	-393.50
Carbon monoxide	-110.52
Naphthalene	151.06

Table 4.12: *Energy balance on Gasifier*

Stream no.	**13**		**21**	
Stream				
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
Carbon	850.94	$\widehat{H1}$	85.09	$\widehat{H7}$
Hydrogen	249.81	$\widehat{H2}$	601.47	$\widehat{H8}$
Oxygen	222.94	$\widehat{H3}$	2.55	$\widehat{H9}$
Nitrogen	12.89	$\widehat{H4}$	12.89	$\widehat{H10}$
Sulfur	8.08	$\widehat{H5}$	0.56	$\widehat{H11}$
Steam	-	-	20.33	$\widehat{H12}$
Hydrogen Sulfide	-	-	7.51	$\widehat{H13}$
Methane	-	-	23.74	$\widehat{H14}$
Carbon dioxide	-	-	118.70	$\widehat{H15}$
Carbon monoxide	-	-	623.39	$\widehat{H16}$
Naphthalene	-	-	0.34	$\widehat{H17}$
Oxygen from ASU	6.69	$\widehat{H6}$	-	-
Ash	-	-	208.40	$\widehat{H18}$
Pressure bar	5		5	
Temperature ºC	250		850	
Reference Temperature ºC	25			

4.4.1. Inlet and outlet enthalpy for gasifier:

Table 4.13: *Inlet and outlet enthalpy for gasifier*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
Carbon	$\boldsymbol{\widehat{H1}}$	5.02
Hydrogen	$\boldsymbol{\widehat{H2}}$	6.50
Oxygen	$\boldsymbol{\widehat{H3}}$	6.87
Nitrogen	$\boldsymbol{\widehat{H4}}$	6.62
Sulfur	$\boldsymbol{\widehat{H5}}$	4.68
Oxygen from ASU[17]	$\boldsymbol{\widehat{H6}}$	27.11

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
Carbon	$\boldsymbol{\widehat{H7}}$	13.76
Hydrogen	$\boldsymbol{\widehat{H8}}$	24.38
Oxygen	$\boldsymbol{\widehat{H9}}$	27.11
Nitrogen	$\boldsymbol{\widehat{H10}}$	25.51
Sulfur	$\boldsymbol{\widehat{H11}}$	21.73
Steam	$\boldsymbol{\widehat{H12}}$	-204.03
H2S	$\boldsymbol{\widehat{H13}}$	13.45
CH4	$\boldsymbol{\widehat{H14}}$	-27.49
CO2	$\boldsymbol{\widehat{H15}}$	-353.36
CO	$\boldsymbol{\widehat{H16}}$	-84.71
Naphthalene (kJ/mol.)	$\boldsymbol{\widehat{H17}}$	436.91
Ash	$\boldsymbol{\widehat{H18}}$	107.48

- Again, it should be observed that heat capacities should be also evaluated in terms of elevated pressures. Now,

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \qquad (4.8)$$

$$\boldsymbol{(\Delta\ H)^{\cdot} = -68402837.46\ kJ/hr}.$$

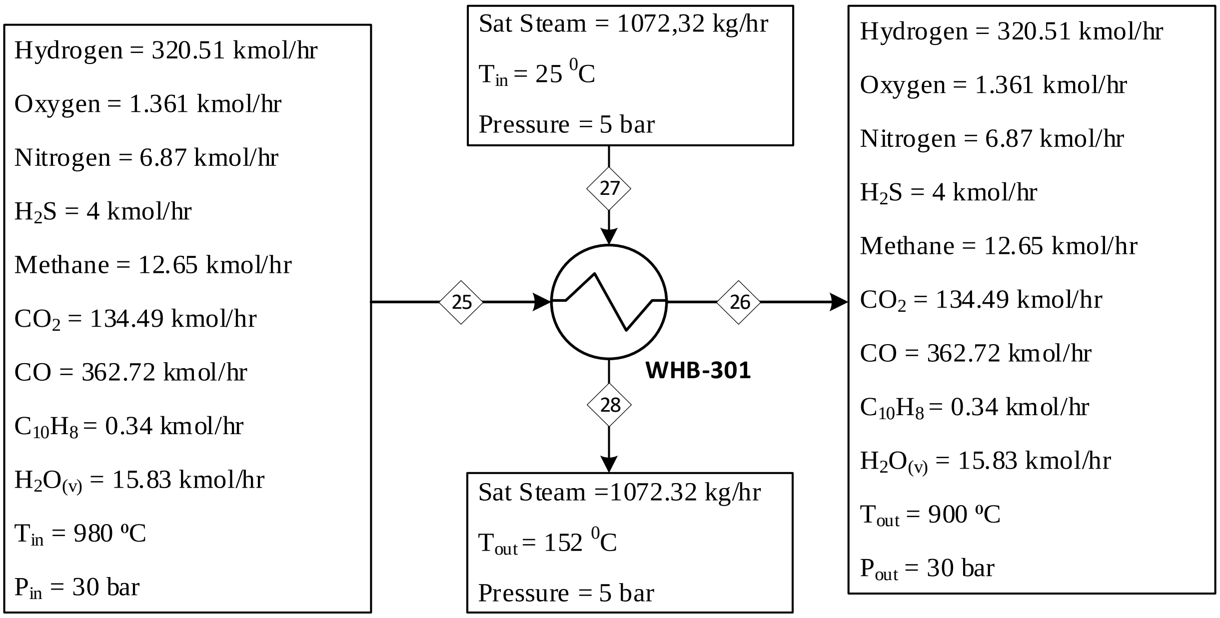
Table 4.14: *Utility requirement*

Utility requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \lambda$	
λ at 10 bars	2013.1 kJ/kg
$\dot{\boldsymbol{m}}$	33978.85 kg/hr.

---

[17] The oxygen entering from ASU is at 850 ºC.

4.5. Energy balance on WHB-301:



Hydrogen = 320.51 kmol/hr
Oxygen = 1.361 kmol/hr
Nitrogen = 6.87 kmol/hr
H_2S = 4 kmol/hr
Methane = 12.65 kmol/hr
CO_2 = 134.49 kmol/hr
CO = 362.72 kmol/hr
$C_{10}H_8$ = 0.34 kmol/hr
$H_2O_{(v)}$ = 15.83 kmol/hr
T_{in} = 980 ºC
P_{in} = 30 bar

Sat Steam = 1072,32 kg/hr
T_{in} = 25 ^{0}C
Pressure = 5 bar

Sat Steam =1072.32 kg/hr
T_{out} = 152 ^{0}C
Pressure = 5 bar

Hydrogen = 320.51 kmol/hr
Oxygen = 1.361 kmol/hr
Nitrogen = 6.87 kmol/hr
H_2S = 4 kmol/hr
Methane = 12.65 kmol/hr
CO_2 = 134.49 kmol/hr
CO = 362.72 kmol/hr
$C_{10}H_8$ = 0.34 kmol/hr
$H_2O_{(v)}$ = 15.83 kmol/hr
T_{out} = 900 ºC
P_{out} = 30 bar

Figure 4.5: *Energy balance on WHB-301*

Table 4.15: *Energy balance on WHB-301*

Stream no.	**25**		**26**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	320.51	$\widehat{H1}$	320.51	$\widehat{H10}$
O_2	1.361	$\widehat{H2}$	1.361	$\widehat{H11}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H12}$
H_2S	4	$\widehat{H4}$	4	$\widehat{H13}$
CH_4	12.65	$\widehat{H5}$	12.65	$\widehat{H14}$
CO_2	134.49	$\widehat{H6}$	134.49	$\widehat{H15}$
CO	362.72	$\widehat{H7}$	362.72	$\widehat{H16}$
$C_{10}H_8$	0.34	$\widehat{H8}$	0.345	$\widehat{H17}$
$H_2O_{(v)}$	15.83	$\widehat{H9}$	15.83	$\widehat{H18}$
Pressure bar	30		30	
Temperature ºC	980.6		900	
Reference Temperature ºC	25			

4.5.1. Inlet and outlet enthalpy on WHB-301:

Table 4.16: *inlet and outlet enthalpy on WHB-301.*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H}1}$	28.43
O_2	$\widehat{\boldsymbol{H}2}$	35.08
N_2	$\widehat{\boldsymbol{H}3}$	33.57
H_2S	$\widehat{\boldsymbol{H}4}$	49.17
CH_4	$\widehat{\boldsymbol{H}5}$	83.16
CO_2	$\widehat{\boldsymbol{H}6}$	55.97
CO	$\widehat{\boldsymbol{H}7}$	33.79
$C_{10}H_8$	$\widehat{\boldsymbol{H}8}$	349.47
$H_2O_{(v)}$	$\widehat{\boldsymbol{H}9}$	45.01

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H}10}$	25.92
O_2	$\widehat{\boldsymbol{H}11}$	31.92
N_2	$\widehat{\boldsymbol{H}12}$	30.50
H_2S	$\widehat{\boldsymbol{H}13}$	44.33
CH_4	$\widehat{\boldsymbol{H}14}$	75
CO_2	$\widehat{\boldsymbol{H}15}$	50.90
CO	$\widehat{\boldsymbol{H}16}$	30.72
$C_{10}H_8$	$\widehat{\boldsymbol{H}17}$	311.22
$H_2O_{(v)}$	$\widehat{\boldsymbol{H}18}$	40.77

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \qquad (4.9)$$

$$(\boldsymbol{\Delta H})^{\cdot} = \boldsymbol{-2828548.374\ kJ/hr}.$$

Table 4.17: *Utility requirement for WHB-301*

Utility requirement	
$\dot{\boldsymbol{Q}} = \dot{\boldsymbol{m}} * \boldsymbol{Cp} * \boldsymbol{\Delta T} + \dot{\boldsymbol{m}} * \boldsymbol{\lambda}$	
Cp at average temperature	4.18 (kJ/kg. ºK)
ΔT	(152-25) ºC
λ at 5 bars	2106.9 kJ/kg
$\dot{\boldsymbol{m}}$	1072.32 kg/hr.

4.6. Energy balance on tar reformer:

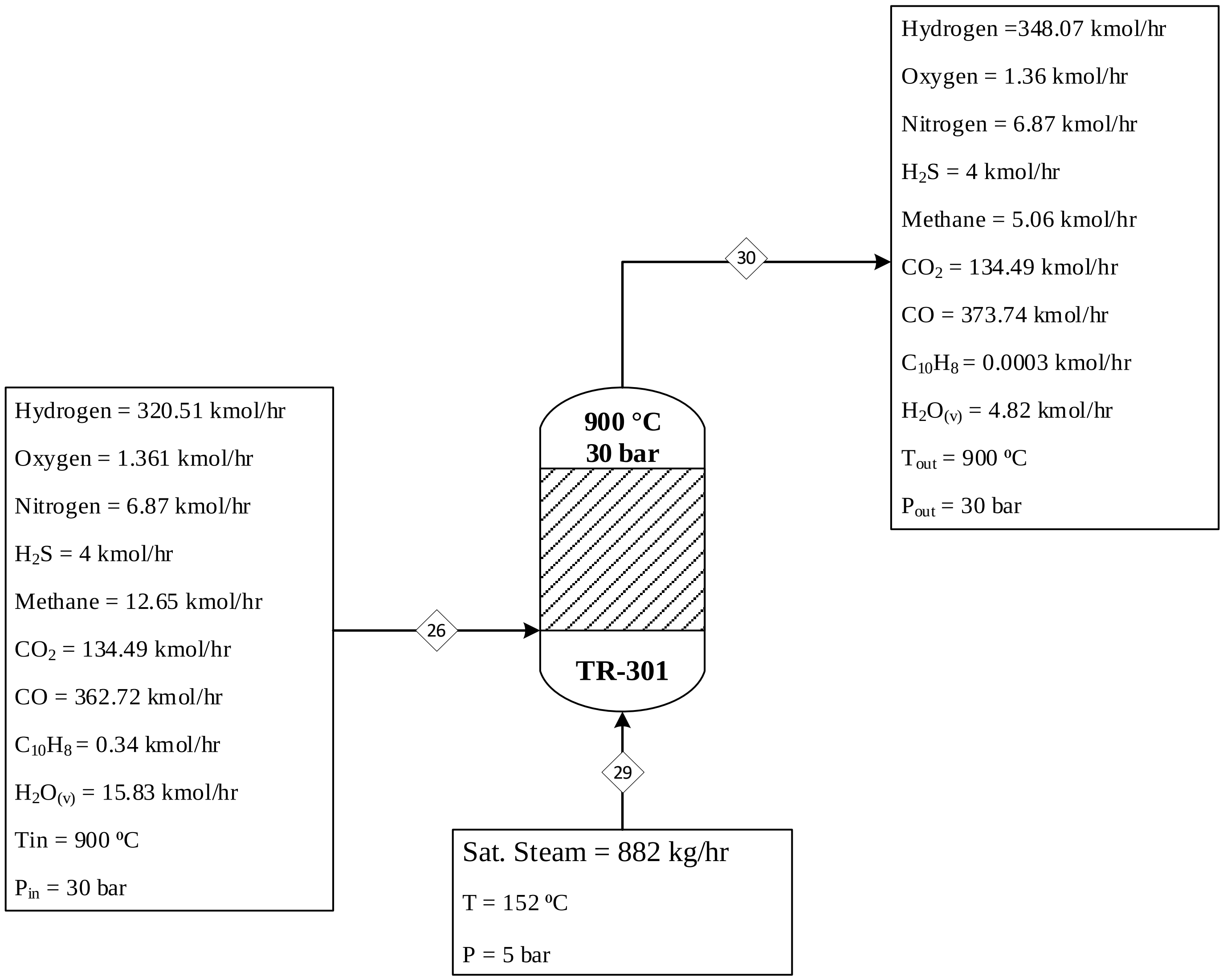


Figure 4.6: *Energy balance on TR-301.*

Heat of formation method is again followed to find out the total enthalpy change due to naphthalene reforming.

Heat of formation of different substances ΔH_f^o	
Components	**ΔH_f^o (kJ/mol.)**
Carbon	0.00
Hydrogen	0.00
Oxygen	0.00
Nitrogen	0.00
Sulfur	0.00
Steam	-241.83
Hydrogen Sulfide	-19.96
Methane	-74.85
Carbon dioxide	-393.50
Carbon monoxide	-110.52
Naphthalene	151.06

Table 4.18: *Energy balance on tar reformer*

Stream no.	**26**		**31**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	320.51	$\widehat{H1}$	348.07	$\widehat{H10}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H11}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H12}$
H_2S	4	$\widehat{H4}$	4	$\widehat{H13}$
CH_4	12.65	$\widehat{H5}$	5.06	$\widehat{H14}$
CO_2	134.49	$\widehat{H6}$	134.49	$\widehat{H15}$
CO	362.72	$\widehat{H7}$	373.74	$\widehat{H16}$
$C_{10}H_8$	0.34	$\widehat{H8}$	0.0003	$\widehat{H17}$
$H_2O_{(v)}$	15.83	$\widehat{H9}$	4.82	$\widehat{H18}$
Pressure (bar)	30		30	
Temperature ºC	900		900	
Reference Temperature ºC	25			

4.6.1. Inlet and outlet enthalpy for tar reformer:

Table 4.19: *inlet and outlet enthalpy for tar reformer*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{H1}$	25.92
O_2	$\widehat{H2}$	28.88
N_2	$\widehat{H3}$	27.18
H_2S	$\widehat{H4}$	24.392
CH_4	$\widehat{H5}$	0.196
CO_2	$\widehat{H6}$	-342.6
CO	$\widehat{H7}$	-83.02
$C_{10}H_8$	$\widehat{H8}$	464.91
$H_2O_{(v)}$	$\widehat{H9}$	-201.05

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H}10}$	25.92
O_2	$\boldsymbol{\widehat{H11}}$	28.88
N_2	$\boldsymbol{\widehat{H12}}$	27.18
H_2S	$\boldsymbol{\widehat{H13}}$	24.392
CH_4	$\boldsymbol{\widehat{H}14}$	0.196
CO_2	$\boldsymbol{\widehat{H15}}$	-342.6
CO	$\boldsymbol{\widehat{H16}}$	-83.02
$C_{10}H_8$	$\boldsymbol{\widehat{H17}}$	464.91
$H_2O_{(v)}$	$\boldsymbol{\widehat{H}18}$	-201.05

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \tag{4.10}$$

$$\boldsymbol{(\Delta\ H)^{\cdot} = +1857306.83\ kJ/hr.}$$

Table 4.20: *Utility requirement for tar reformer*

Utility requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \lambda$	
λ at 5 bars	2106.9 kJ/kg
$\dot{\boldsymbol{m}}$	882 kg/hr.

4.7. Energy balance on WHB-302:

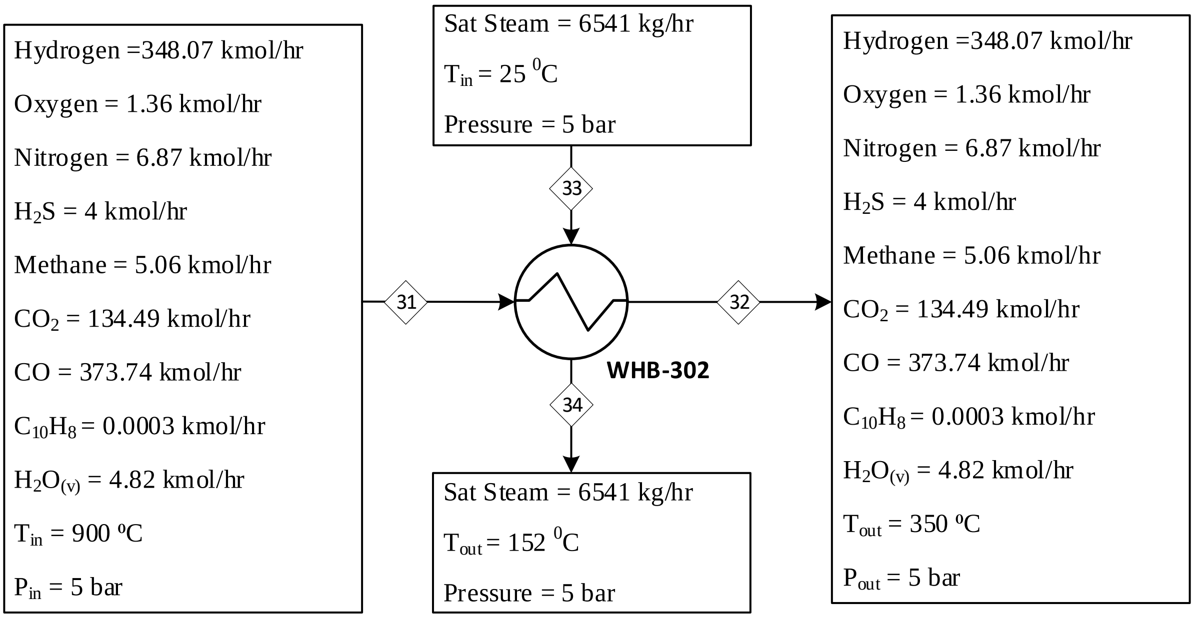


Figure 4.7: *Energy balance on WHB-302.*

Table 4.21: *Energy balance on WHB-302*

Stream no.	**31**		**32**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	348.07	$\widehat{H}1$	348.07	$\widehat{H}10$
O_2	1.361	$\widehat{H2}$	1.361	$\widehat{H11}$
N_2	6.871	$\widehat{H3}$	6.871	$\widehat{H12}$
H_2S	4	$\widehat{H4}$	4	$\widehat{H13}$
CH_4	5.06	$\widehat{H5}$	5.06	$\widehat{H14}$
CO_2	134.49	$\widehat{H6}$	134.49	$\widehat{H15}$
CO	373.74	$\widehat{H7}$	373.74	$\widehat{H16}$
$C_{10}H_8$	0.0034	$\widehat{H8}$	0.00034	$\widehat{H17}$
$H_2O_{(v)}$	4.82	$\widehat{H9}$	4.82	$\widehat{H}18$
Pressure bar	5		5	
Temperature ºC	900		350	
Reference Temperature ºC	25			

4.7.1. Inlet and outlet enthalpy for WHB-302:

Table 4.22: *Inlet and outlet enthalpy for whb-302.*

Enthalpies of inlet stream		
Component	**Enthalpies (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H}\mathbf{1}}$	25.92
O_2	$\widehat{\boldsymbol{H}\mathbf{2}}$	28.88
N_2	$\widehat{\boldsymbol{H}\mathbf{3}}$	27.18
H_2S	$\widehat{\boldsymbol{H}\mathbf{4}}$	44.35
CH_4	$\widehat{\boldsymbol{H}\mathbf{5}}$	75.04
CO_2	$\widehat{\boldsymbol{H}\mathbf{6}}$	50.89
CO	$\widehat{\boldsymbol{H}\mathbf{7}}$	27.49
$C_{10}H_8$	$\widehat{\boldsymbol{H}\mathbf{8}}$	309.21
$H_2O_{(v)}$	$\widehat{\boldsymbol{H}\mathbf{9}}$	40.48

Enthalpies of outlet stream		
Component	**Enthalpies (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H}\mathbf{10}}$	9.42
O_2	$\widehat{\boldsymbol{H}\mathbf{11}}$	10.08
N_2	$\widehat{\boldsymbol{H}\mathbf{12}}$	9.62
H_2S	$\widehat{\boldsymbol{H}\mathbf{13}}$	14.24
CH_4	$\widehat{\boldsymbol{H}\mathbf{14}}$	21.83
CO_2	$\widehat{\boldsymbol{H}\mathbf{15}}$	17.29
CO	$\widehat{\boldsymbol{H}\mathbf{16}}$	10.55
$C_{10}H_8$	$\widehat{\boldsymbol{H}\mathbf{17}}$	83.62
$H_2O_{(v)}$	$\widehat{\boldsymbol{H}\mathbf{18}}$	13.23

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \qquad (4.11)$$

$$(\boldsymbol{\Delta}\ \boldsymbol{H})^{\cdot} = \mathbf{-17261776.8}\ \boldsymbol{kJ/hr}.$$

Table 4.23: *Utility requirement for WHB-302*

Utility requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \boldsymbol{Cp} * \boldsymbol{\Delta T} + \dot{\mathbf{m}} * \lambda$	
Cp at average temperature	4.19 (kJ/kg. ºK)
ΔT	(152-25) ºC
λ at 5 bars	2106.9 kJ/kg
$\dot{\boldsymbol{m}}$	6541 kg/hr.

4.8. Energy balance on water gas shift reactor (R-301):

Heat of reaction method was followed here to find the total enthalpy change,

$$Specific\ enthalpy\ changes\ or\ \boldsymbol{\widehat{H}} = \int_{Tr}^{T} \boldsymbol{a} + \int_{Tr}^{T} \boldsymbol{bT} + \int_{Tr}^{T} \boldsymbol{cT^2} + \int_{Tr}^{T} \boldsymbol{dT^3} \tag{4.12}$$

$$Total\ Enthalpy\ Change, \Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\varepsilon} * \Delta H_{ro} \tag{4.13}$$

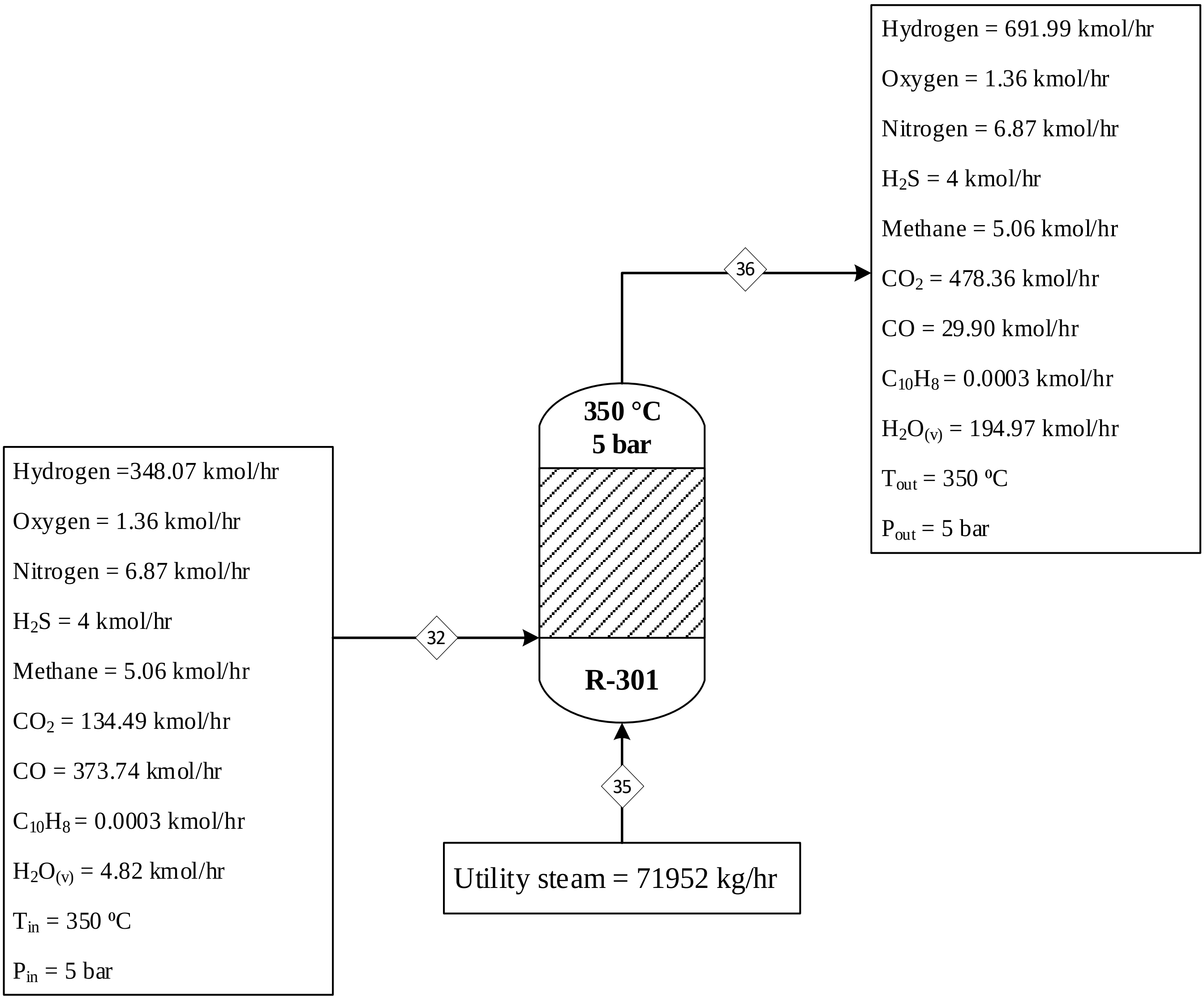


Figure 4.8: *Energy balance on R-301.*

Table 4.24: *Energy balance on WGS reactor*

Stream no.	**32**		**36**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	348	$\widehat{\boldsymbol{H1}}$	691.99	$\widehat{\boldsymbol{H10}}$
O_2	1.36	$\widehat{\boldsymbol{H2}}$	1.36	$\widehat{\boldsymbol{H11}}$
N_2	6.87	$\widehat{\boldsymbol{H3}}$	6.87	$\widehat{\boldsymbol{H12}}$
H_2S	4	$\widehat{\boldsymbol{H4}}$	4	$\widehat{\boldsymbol{H13}}$
CH_4	5.06	$\widehat{\boldsymbol{H5}}$	5.06	$\widehat{\boldsymbol{H14}}$
CO_2	134.49	$\widehat{\boldsymbol{H6}}$	478.36	$\widehat{\boldsymbol{H15}}$
CO	373.74	$\widehat{\boldsymbol{H7}}$	29.90	$\widehat{\boldsymbol{H16}}$
$H_2O_{(v)}$	4.78	$\widehat{\boldsymbol{H8}}$	194.97	$\widehat{\boldsymbol{H17}}$
$C_{10}H_8$	0.0003	$\widehat{\boldsymbol{H9}}$	0.0003	$\widehat{\boldsymbol{H18}}$
Pressure	5		5	
Temperature ^{0}C	350		350	
Reference Temperature ^{0}C	25			

4.8.1. Inlet and outlet enthalpy for WGS reactor

Table 4.25: *Inlet and outlet enthalpy for WGS reactor*

Enthalpies of inlet stream		
Component	**Enthalpies (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H1}}$	9.421
O_2	$\widehat{\boldsymbol{H2}}$	10.08
N_2	$\widehat{\boldsymbol{H3}}$	9.62
H_2S	$\widehat{\boldsymbol{H4}}$	14.24
CH_4	$\widehat{\boldsymbol{H5}}$	21.83
CO_2	$\widehat{\boldsymbol{H6}}$	17.29
CO	$\widehat{\boldsymbol{H7}}$	10.55
$H_2O_{(v)}$	$\widehat{\boldsymbol{H8}}$	13.20
$C_{10}H_8$	$\widehat{\boldsymbol{H9}}$	87.13

Enthalpies of outlet stream		
Component	**Enthalpies (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H}10}$	9.421
O_2	$\widehat{\boldsymbol{H}11}$	10.08
N_2	$\widehat{\boldsymbol{H}12}$	9.62
H_2S	$\widehat{\boldsymbol{H}13}$	14.24
CH_4	$\widehat{\boldsymbol{H}14}$	21.83
CO_2	$\widehat{\boldsymbol{H}15}$	17.29
CO	$\widehat{\boldsymbol{H}16}$	10.55
$H_2O_{(v)}$	$\widehat{\boldsymbol{H}17}$	13.20
$C_{10}H_8$	$\widehat{\boldsymbol{H}18}$	87.13

Heat of reaction, ΔH_r^o = -41 kJ/mol.

Extent of reaction based on CO = 343.8418371

$$Total\ Enthalpy\ Change, \Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\varepsilon} * \Delta H_r o$$

$$(\boldsymbol{\Delta H})^{\cdot} = \boldsymbol{-6029565.29\ kJ/hr}.$$

Table 4.26: *utility requirement for WGS reactor*

Utility requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * Cp * \boldsymbol{\Delta T}$	
$\boldsymbol{\Delta T}$	20
$\dot{\boldsymbol{m}}$	71952 kg/hr.

4.9. Energy balance on WHB-303:

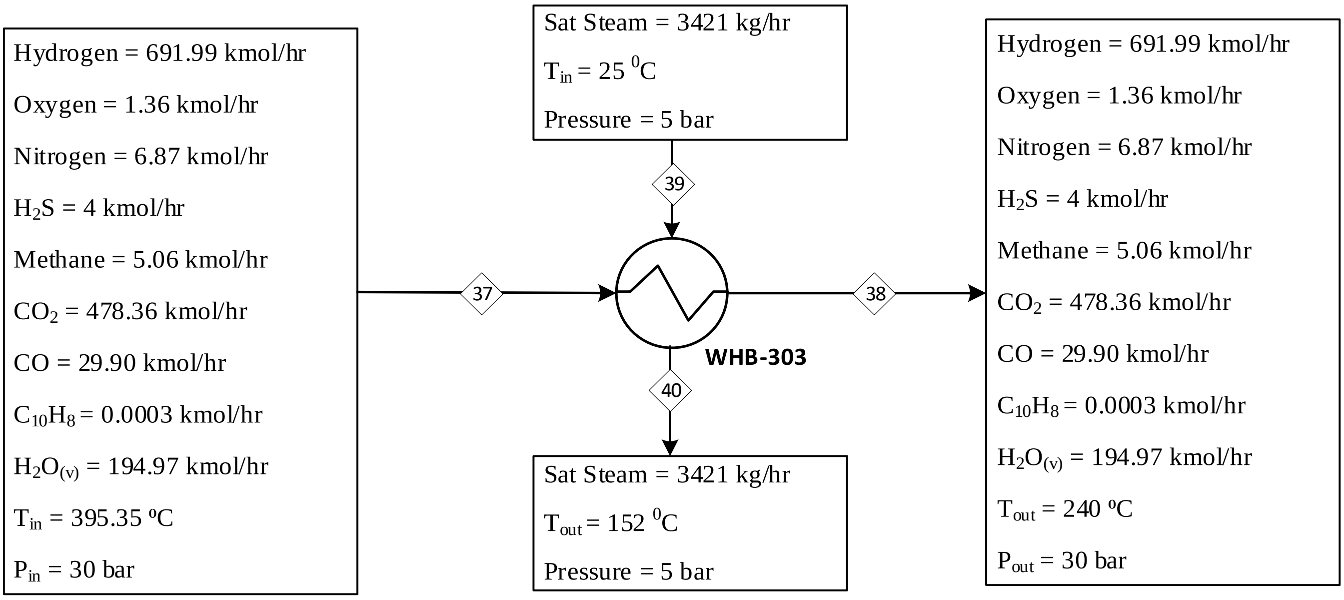


Figure 4.9: *Energy balance on WHB-302.*

Table 4.27: *Energy balance on WHB-303*

Stream no.	**37**		**38**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol)**
H_2	691.99	$\widehat{\boldsymbol{H}}\mathbf{1}$	691.99	$\widehat{\boldsymbol{H}}\mathbf{10}$
O_2	1.36	$\widehat{\boldsymbol{H}}\mathbf{2}$	1.36	$\widehat{\boldsymbol{H}}\mathbf{11}$
N_2	6.87	$\widehat{\boldsymbol{H}}\mathbf{3}$	6.87	$\widehat{\boldsymbol{H}}\mathbf{12}$
H_2S	4	$\widehat{\boldsymbol{H}}\mathbf{4}$	4	$\widehat{\boldsymbol{H}}\mathbf{13}$
CH_4	5.06	$\widehat{\boldsymbol{H}}\mathbf{5}$	5.06	$\widehat{\boldsymbol{H}}\mathbf{14}$
CO_2	478.36	$\widehat{\boldsymbol{H}}\mathbf{6}$	478.36	$\widehat{\boldsymbol{H}}\mathbf{15}$
CO	29.9	$\widehat{\boldsymbol{H}}\mathbf{7}$	29.9	$\widehat{\boldsymbol{H}}\mathbf{16}$
$H_2O_{(v)}$	194.97	$\widehat{\boldsymbol{H}}\mathbf{8}$	194.97	$\widehat{\boldsymbol{H}}\mathbf{17}$
$C_{10}H_8$	0.0003	$\widehat{\boldsymbol{H}}\mathbf{9}$	0.0003	$\widehat{\boldsymbol{H}}\mathbf{18}$
Pressure bar	30		30	
Temperature °C	395.35		240	
Reference Temperature °C	25			

4.9.1. Inlet and outlet enthalpy of WHB-303:

Table 4.28: *Inlet and outlet enthalpy of WHB-303*

Enthalpies of inlet stream		
Component	**Enthalpies (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H1}}$	10.74
O_2	$\boldsymbol{\widehat{H2}}$	12.85
N_2	$\boldsymbol{\widehat{H3}}$	11.98
H_2S	$\boldsymbol{\widehat{H4}}$	17.04
CH_4	$\boldsymbol{\widehat{H5}}$	25.79
CO_2	$\boldsymbol{\widehat{H6}}$	20.30
CO	$\boldsymbol{\widehat{H7}}$	12.15
$H_2O_{(v)}$	$\boldsymbol{\widehat{H8}}$	17.91
$C_{10}H_8$	$\boldsymbol{\widehat{H9}}$	104.73

Enthalpies of outlet stream		
Component	**Enthalpies (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H10}}$	6.21
O_2	$\boldsymbol{\widehat{H11}}$	7.31
N_2	$\boldsymbol{\widehat{H12}}$	6.77
H_2S	$\boldsymbol{\widehat{H13}}$	10.31
CH_4	$\boldsymbol{\widehat{H14}}$	13.49
CO_2	$\boldsymbol{\widehat{H15}}$	11.66
CO	$\boldsymbol{\widehat{H16}}$	6.90
$H_2O_{(v)}$	$\boldsymbol{\widehat{H17}}$	10.42
$C_{10}H_8$	$\boldsymbol{\widehat{H18}}$	52.19

$$Total\ Enthalpy\ Change, \Delta\ H\ =\ \Sigma(n_iH_i)_{prod}\ -\ \Sigma(n_iH_i)_{react} \qquad (4.14)$$

$$\boldsymbol{(\Delta\ H)^{\cdot}\ =\ -9023137.485\ kJ/hr.}$$

Table 4.29: *Utility requirement for WHB-303*

Utility requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \boldsymbol{Cp} * \boldsymbol{\Delta T} + \dot{\mathbf{m}} *\lambda$	
Cp at average temperature	4.18(kJ/kg. ºK)
ΔT	(127) ºC
λ at 5 bars	2106.9 kJ/kg
$\dot{\boldsymbol{m}}$	3421 kg/hr.

4.10. Energy balance on ST-301:

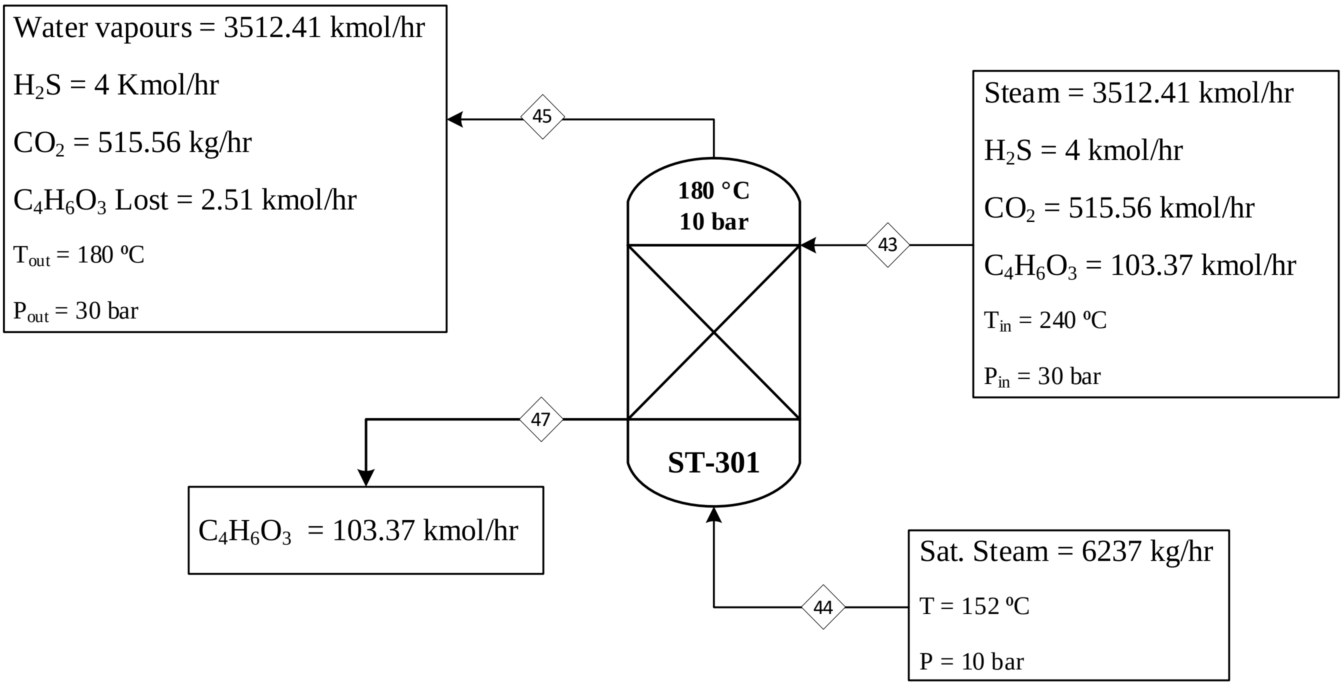


Figure 4.10: Energy balance on stripper (ST-301).

Table 4.30: Energy balance on ST-301

Stream no.	**43**		**45**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
CO_2	515.56	$\widehat{H1}$	515.56	$\widehat{H5}$
H_2S	4	$\widehat{H2}$	4	$\widehat{H6}$
$C_4H_6O_3$	103.37	$\widehat{H3}$	103.37	$\widehat{H7}$
$C_4H_6O_3$ Lost	-	-	2.51	$\widehat{H8}$
$H_2O_{(v)}$	3512.41	$\widehat{H4}$	3512.41	$\widehat{H9}$
Pressure bar	30		30	
Temperature ºC	240		180	
Reference Temperature ºC	25			

- Lean solvent outlet temperature was found via an iterative method. By considering the fact that inlet enthalpies must balance the outlet enthalpies the outlet temperature of solvent was found to be 417 ºC.

4.10.1. Inlet and outlet enthalpy of ST-301:

Table 4.31: *Inlet and outlet enthalpy of ST-301*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
CO_2	$\widehat{\boldsymbol{H1}}$	11.83
H_2S	$\widehat{\boldsymbol{H2}}$	10.59
$C_4H_6O_3$	$\widehat{\boldsymbol{H3}}$	31.16
$H_2O_{(v)}$	$\widehat{\boldsymbol{H4}}$	11.07

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
CO_2	$\widehat{\boldsymbol{H5}}$	7.89
H_2S	$\widehat{\boldsymbol{H6}}$	6.79
$C_4H_6O_3$[18]	$\widehat{\boldsymbol{H7}}$	70.56
$C_4H_6O_3$ Lost	$\widehat{\boldsymbol{H8}}$	22.47
$H_2O_{(v)}$	$\widehat{\boldsymbol{H9}}$	6.94

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_iH_i)_{prod} - \Sigma(n_iH_i)_{react} \tag{4.15}$$

$$(\boldsymbol{\Delta H})^{\cdot} = \boldsymbol{-12596011\ kJ/hr}.$$

Table 4.32: *Utility requirement for ST-301*

Utility requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \lambda$	
λ at 10 bars	2013.1 kJ/kg
$\dot{\boldsymbol{m}}$	6257 kg/hr.

---

[18] Outlet temperature is 417**°C**

4.11. Energy balance on WHB-304:

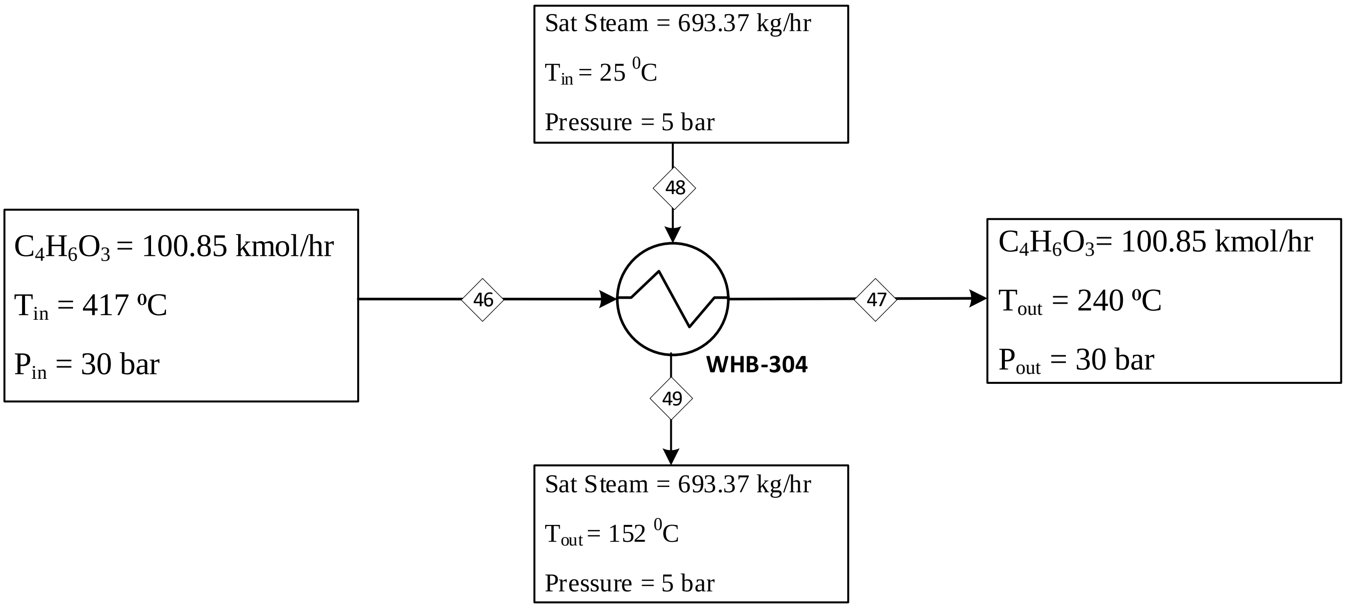


Figure 4.11: *Energy balance on WHB-304.*

Table 4.33: *Energy balance on WHB-304*

Stream no.	**46**		**47**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
$C_4H_6O_3$	100.85	$\boldsymbol{\widehat{H1}}$	100.85	$\boldsymbol{\widehat{H2}}$
Pressure bar	30		30	
Temperature ^{o}C	417		240	
Reference Temperature ^{o}C	25			

4.11.1. Inlet and outlet enthalpy of WHB-304

Table 4.34: *Inlet and outlet enthalpy of WHB-304*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
$C_4H_6O_3$	$\boldsymbol{\widehat{H1}}$	56.834
Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
$C_4H_6O_3$	$\boldsymbol{\widehat{H2}}$	38.7

$$Total\ Enthalpy\ Change, \Delta\ H\ =\ \Sigma(n_iH_i)_{prod}\ -\ \Sigma(n_iH_i)_{react} \qquad (4.16$$

$$\boldsymbol{(\Delta\ H)^{\cdot}\ =\ -1828946\ kJ/hr.}$$

Table 4.35: *Utility requirement for WHB-304*

Utility requirement	
As, $\dot{Q} = \dot{m} * Cp * \Delta T + \dot{m} * \lambda$	
ΔT	127
Cp at average temperature	4.18
λ	2106.9
$\dot{m}$	693.37 kg/hr.

4.12. Energy balance on E-401:

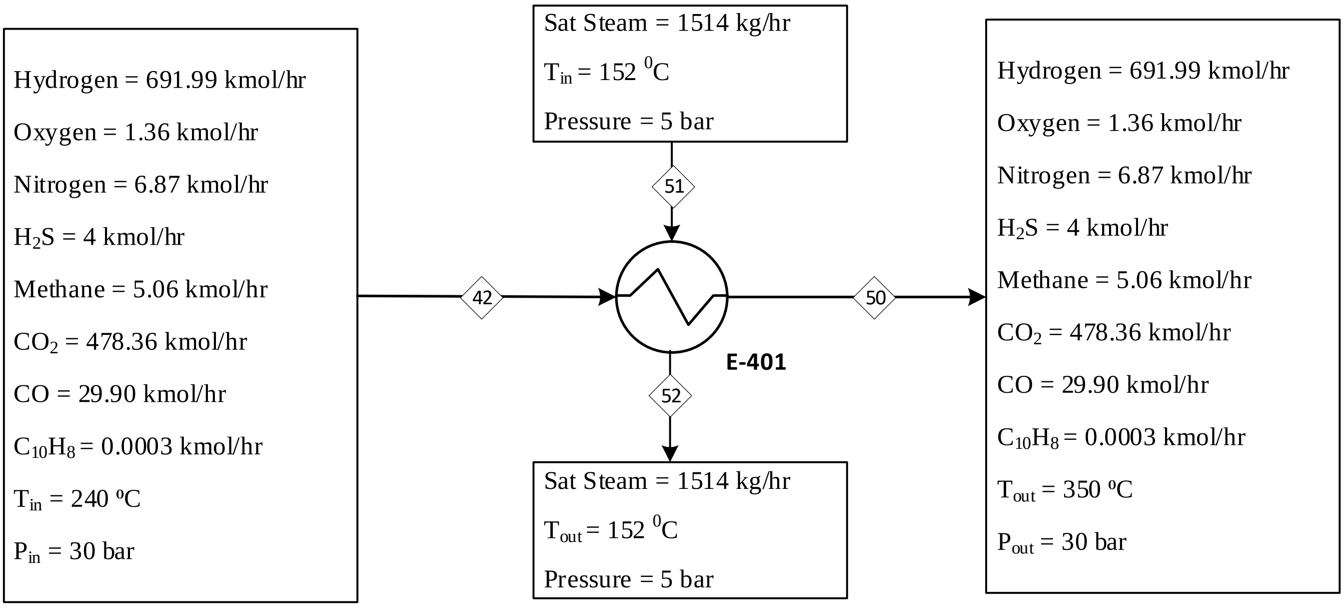


Figure 4.12: *Energy balance on E-401.*

Table 4.36: *Energy balance on E-401*

Stream no.	**42**		**50**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	691.99	$\widehat{H1}$	691.99	$\widehat{H8}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H9}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H10}$
CH_4	5.06	$\widehat{H4}$	5.06	$\widehat{H11}$
CO_2	150.20	$\widehat{H5}$	150.20	$\widehat{H12}$
CO	29.9	$\widehat{H6}$	29.9	$\widehat{H13}$
$C_{10}H_8$	0.00034	$\widehat{H7}$	0.00034	$\widehat{H14}$
Pressure bar	30		30	
Temperature ºC	240		350	
Reference Temperature ºC	25			

4.12.1. Inlet and outlet enthalpy of E-401:

Table 4.37: *Inlet and outlet enthalpy of E-401*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{H1}$	6.21
O_2	$\widehat{H2}$	7.32
N_2	$\widehat{H3}$	6.32
CH_4	$\widehat{H4}$	13.48
CO_2	$\widehat{H5}$	11.87
CO	$\widehat{H6}$	6.90
$C_{10}H_8$	$\widehat{H7}$	6.58

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{H8}$	9.42
O_2	$\widehat{H9}$	10.08
N_2	$\widehat{H10}$	9.62
CH_4	$\widehat{H11}$	21.85
CO_2	$\widehat{H12}$	17.33
CO	$\widehat{H13}$	9.70
$C_{10}H_8$	$\widehat{H14}$	20.87

$$Total\ Enthalpy\ Change, \Delta\ H\ =\ \Sigma(n_i H_i)_{prod}\ -\ \Sigma(n_i H_i)_{react} \qquad (4.17)$$

$$(\boldsymbol{\Delta\ H})^{\cdot}\ =\ \mathbf{3189768}\ \boldsymbol{kJ/hr}.$$

Table 4.38: *Utility requirement for E-401*

Utility requirement	
As, $\dot{Q} = \dot{m} * \lambda$	
λ	2106.9 (kJ/kg)
$\dot{m}$	1514 kg/hr.

4.13. Energy balance on methanator (01):

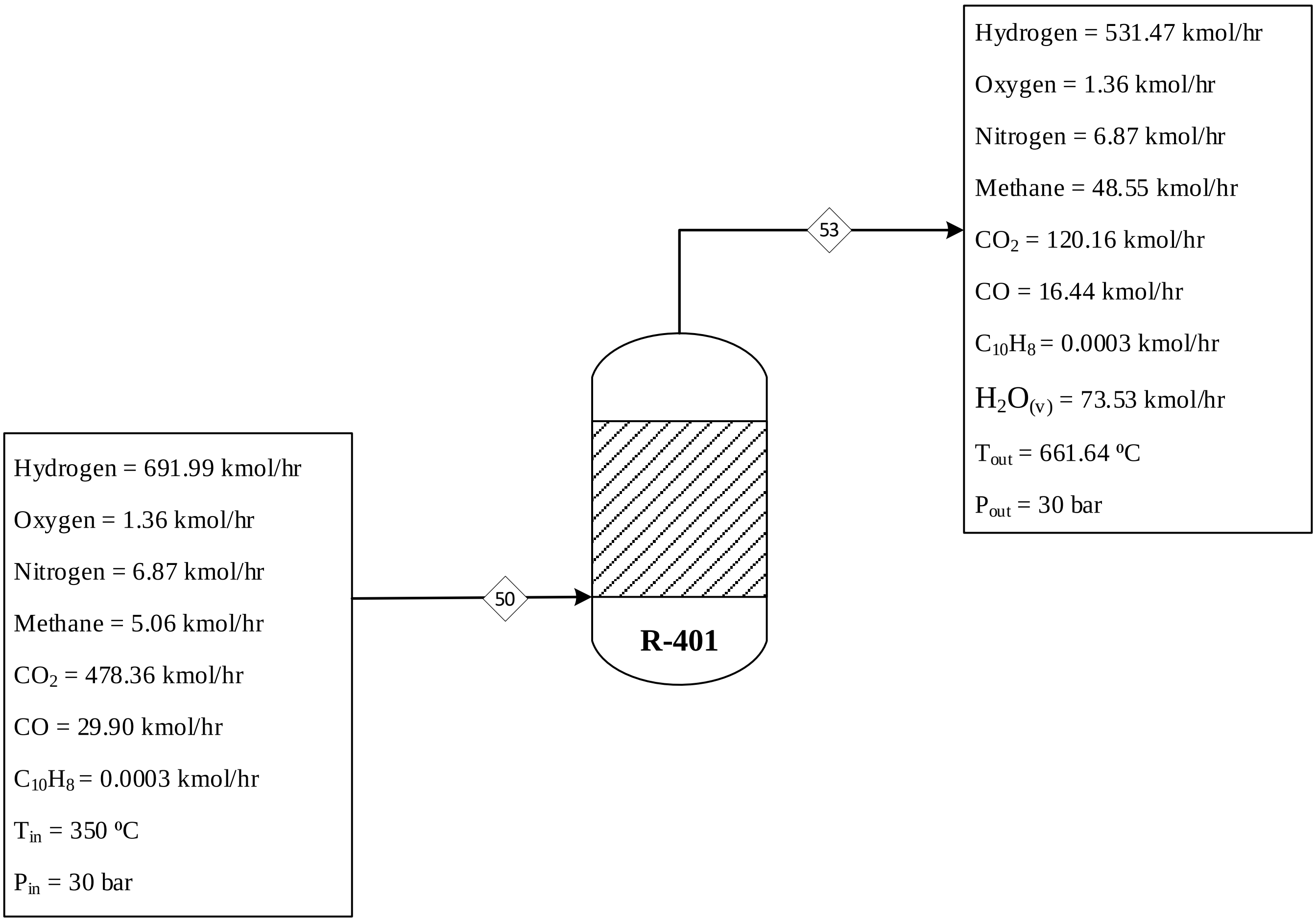


Figure 4.13: *Energy balance on R-401.*

Table 4.39: *Energy balance on methanator -1*

Stream no.	**50**		**53**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	691.99	$\widehat{H1}$	531.46	$\widehat{H9}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H10}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H11}$
CH_4	5.06	$\widehat{H4}$	48.55	$\widehat{H12}$
CO_2	150.20	$\widehat{H5}$	120.16	$\widehat{H13}$
CO	29.90	$\widehat{H6}$	16.44	$\widehat{H14}$
$H_2O_{(v)}$	-	$\widehat{H7}$	73.53	$\widehat{H15}$
$C_{10}H_8$	0.00034	$\widehat{H8}$	0.00034	$\widehat{H16}$
Pressure bar	30		30	
Temperature ºC	350		661.64	
Reference Temperature ºC	25			

- Heat of reaction method was followed for solving for adiabatic temperature rise in methanation reactor.

$$Specific\ enthalpy\ changes\ or\ \boldsymbol{\hat{H}} = \int_{Tr}^{T} \boldsymbol{a} + \int_{Tr}^{T} \boldsymbol{bT} + \int_{Tr}^{T} \boldsymbol{cT^2} + \int_{Tr}^{T} \boldsymbol{dT^3} \qquad (4.18)$$

$$Total\ Enthalpy\ Change, \Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\varepsilon} * \Delta H_{ro} \qquad (4.19)$$

- In an adiabatic reactor the outlet temperature is normally the desired entity to be found by energy balance. The outlet was found via solving the equation given below,

$$Total\ Enthalpy\ Change, \Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\varepsilon} * \Delta H_{ro}$$

- Where $\Delta H = 0$ for adiabatic. The equation becomes,

$$\boldsymbol{\Sigma\varepsilon} * \Delta H_{ro} = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react})$$

The term $(n_i H_i)_{prod}$ is expanded, and the above equation was rearranged in terms of outlet temperature. Now, solving for the outlet temperature yields,

$$\boldsymbol{T_{out} = 661.64\ ^0C}$$

4.13.1. Inlet and outlet enthalpy of methanator-01:

Table 4.40: *Inlet and outlet enthalpy of methanator-01*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H1}}$	9.42
O_2	$\boldsymbol{\widehat{H2}}$	9.62
N_2	$\boldsymbol{\widehat{H3}}$	9.42
CH_4	$\boldsymbol{\widehat{H4}}$	21.85
CO_2	$\boldsymbol{\widehat{H5}}$	17.33
CO	$\boldsymbol{\widehat{H6}}$	9.70
$C_{10}H_8$	$\boldsymbol{\widehat{H8}}$	20.87

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H9}}$	18.65
O_2	$\boldsymbol{\widehat{H10}}$	20.53
N_2	$\boldsymbol{\widehat{H11}}$	19.35
CH_4	$\boldsymbol{\widehat{H12}}$	33.62
CO_2	$\boldsymbol{\widehat{H13}}$	36.05
CO	$\boldsymbol{\widehat{H14}}$	19.56
$H_2O_{(v)}$	$\boldsymbol{\widehat{H15}}$	27.98
$C_{10}H_8$	$\boldsymbol{\widehat{H16}}$	88.64

- In the adiabatic reactor, our main objective is to find the temperature rise of the outlet stream. So, calculation of total enthalpy change was avoided because there is no logical reason to calculate it.

4.14. Energy balance on WHB-401:

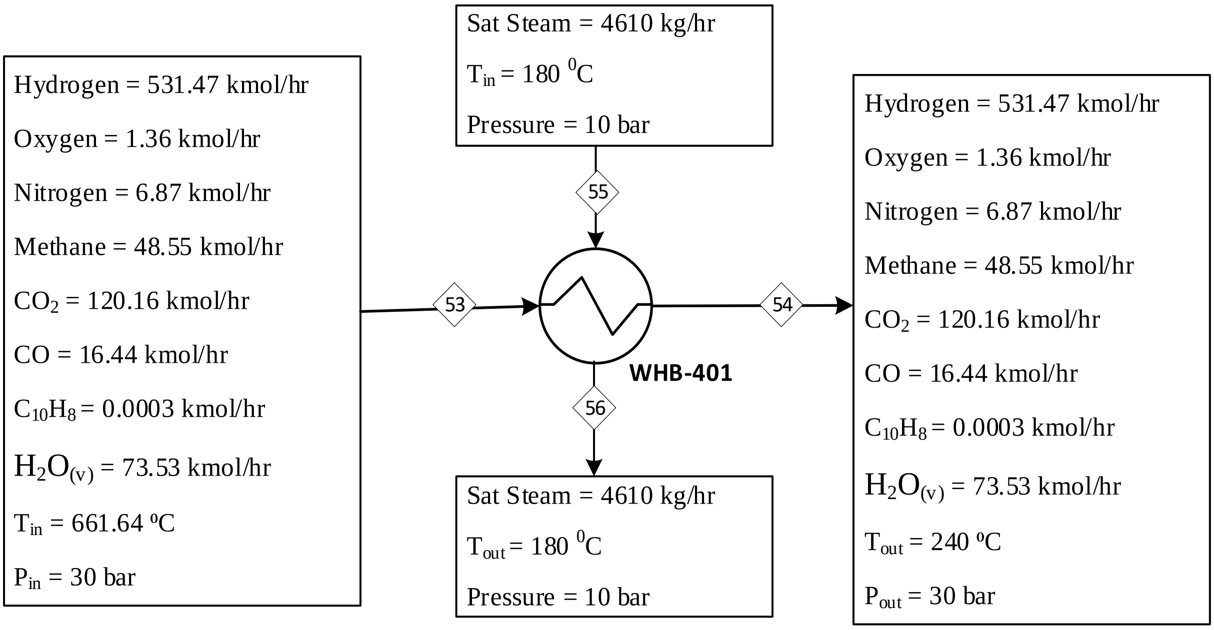


Figure 4.14: *Energy balance on WHB-401.*

Table 4.41: *Energy balance on WHB-401*

Stream no.	**53**		**54**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	531.46	$\widehat{H1}$	531.46	$\widehat{H9}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H10}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H11}$
CH_4	48.55	$\widehat{H4}$	48.55	$\widehat{H12}$
CO_2	120.16	$\widehat{H5}$	120.16	$\widehat{H13}$
CO	16.44	$\widehat{H6}$	16.44	$\widehat{H14}$
$H_2O_{(v)}$	73.53	$\widehat{H7}$	73.53	$\widehat{H15}$
$C_{10}H_8$	0.00034	$\widehat{H8}$	0.00034	$\widehat{H16}$
Pressure bar	30		30	
Temperature ^{o}C	661.64		240	
Reference Temperature ^{o}C	25			

4.14.1. Inlet and outlet enthalpy of WHB-401

Table 4.42: *Inlet and outlet enthalpy of WHB-401*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{H1}$	18.65
O_2	$\widehat{H2}$	20.53
N_2	$\widehat{H3}$	19.35
CH_4	$\widehat{H4}$	33.62
CO_2	$\widehat{H5}$	36.05
CO	$\widehat{H6}$	19.56
$H_2O_{(v)}$	$\widehat{H7}$	27.98
$C_{10}H_8$	$\widehat{H8}$	88.64

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{H9}$	6.21
O_2	$\widehat{H10}$	7.25
N_2	$\widehat{H11}$	6.32
CH_4	$\widehat{H12}$	13.36
CO_2	$\widehat{H13}$	11.14
CO	$\widehat{H14}$	6.83
$H_2O_{(v)}$	$\widehat{H15}$	9.35
$C_{10}H_8$	$\widehat{H16}$	6.58

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \qquad (4.20)$$

$$(\boldsymbol{\Delta H})^{\cdot} = \boldsymbol{-12273492.26\ kJ/hr}.$$

Table 4.43: *Utility requirement for WHB-401*

Utility requirement	
As, $\dot{Q} = \dot{m} * Cp * \Delta T + \dot{m} * \lambda$	
Cp at average temperature	4.19 (kJ/kg. ^oK)
ΔT	(180-25) ^oC
λ at 10 bars	2013.1 kJ/kg
$\dot{m}$	4610 kg/hr.

4.15. Energy balance on methanator (02):

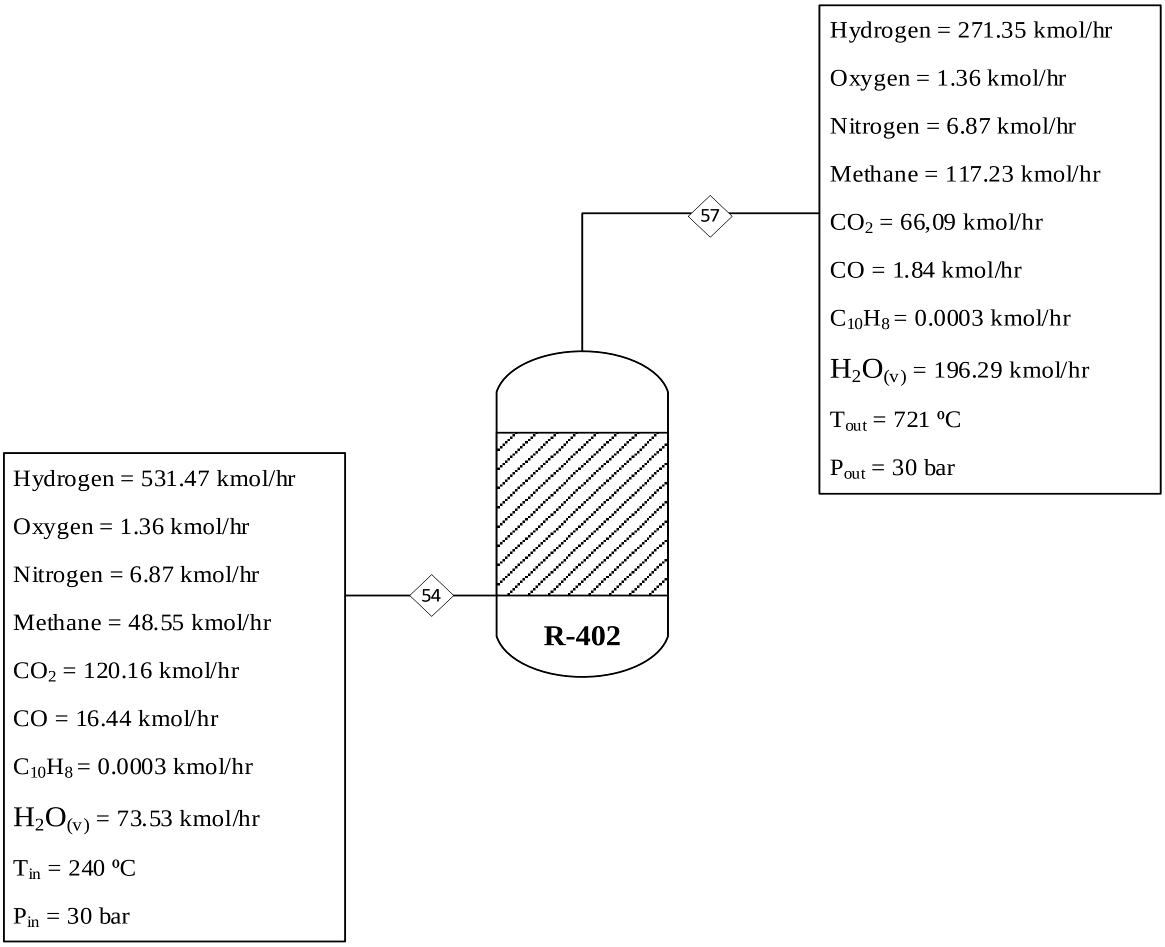


Figure 4.15: *Energy balance on R-402.*

Table 4.44: *Energy balance on methanator-02*

Stream no.	**54**		**57**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	531.46	$\widehat{H1}$	271.35	$\widehat{H9}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H10}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H11}$
CH_4	48.55	$\widehat{H4}$	117.23	$\widehat{H12}$
CO_2	120.16	$\widehat{H5}$	66.09	$\widehat{H13}$
CO	16.44	$\widehat{H6}$	1.84	$\widehat{H14}$
$H_2O_{(v)}$	73.53	$\widehat{H7}$	196.29	$\widehat{H15}$
$C_{10}H_8$	0.00034	$\widehat{H8}$	0.00034	$\widehat{H16}$
Pressure bar	30		30	
Temperature °C	240		721	
Reference Temperature °C	25			

4.15.1. Inlet and outlet enthalpy of methanator-02

- Again, adiabatic temperature rise was found through following formula,

$$\Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\Sigma\varepsilon}^{19} * \Delta H_{ro} \qquad (4.21)$$

Table 4.45: *Inlet and outlet enthalpy of Methanator-02*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H1}}$	6.21
O_2	$\widehat{\boldsymbol{H2}}$	6.55
N_2	$\widehat{\boldsymbol{H3}}$	6.32
CH_4	$\widehat{\boldsymbol{H4}}$	8.94
CO_2	$\widehat{\boldsymbol{H5}}$	8.84
CO	$\widehat{\boldsymbol{H6}}$	6.35
$H_2O_{(v)}$	$\widehat{\boldsymbol{H7}}$	7.42
$C_{10}H_8$	$\widehat{\boldsymbol{H8}}$	6.58

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H9}}$	20.44
O_2	$\widehat{\boldsymbol{H10}}$	22.58
N_2	$\widehat{\boldsymbol{H11}}$	21.27
CH_4	$\widehat{\boldsymbol{H12}}$	37.78
CO_2	$\widehat{\boldsymbol{H13}}$	33.01
CO	$\widehat{\boldsymbol{H14}}$	21.50
$H_2O_{(v)}$	$\widehat{\boldsymbol{H15}}$	25.77
$C_{10}H_8$	$\widehat{\boldsymbol{H16}}$	104.82

$$\boldsymbol{T_{adiabatic} = 721\ {}^{0}C}$$

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[19] Summation for both reactions

4.16. Energy balance on WHB-402:

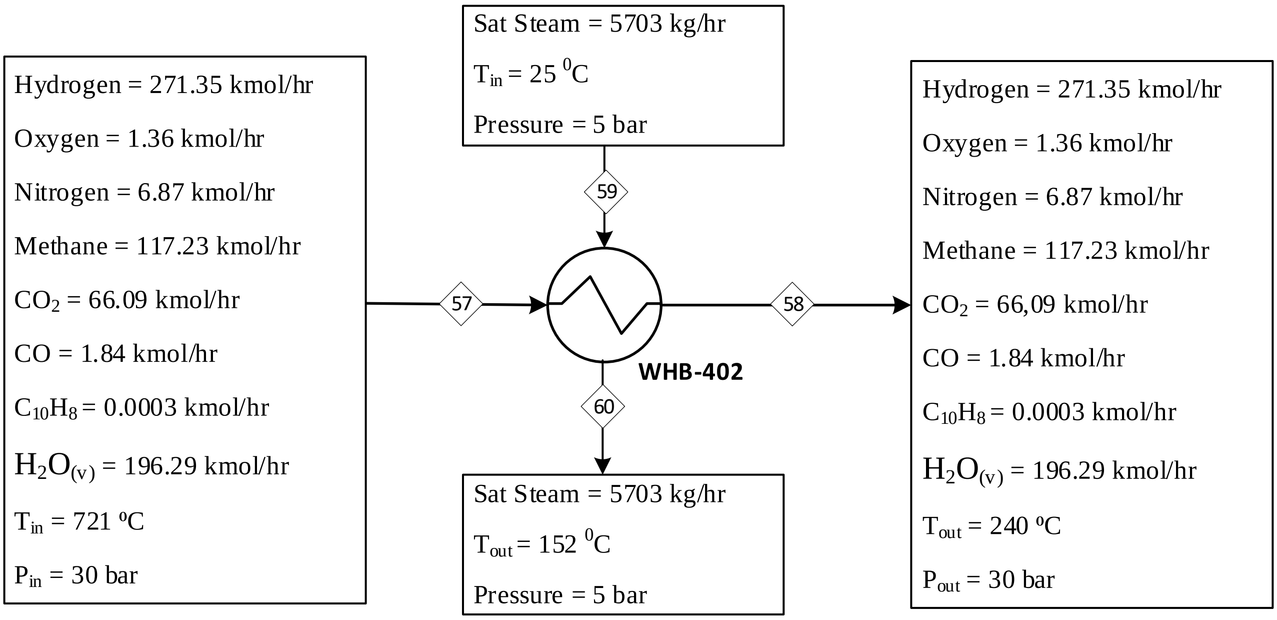

Figure 4.16: *Energy balance on WHB-402.*

Table 4.46: *Energy balance on WHB-402*

Stream no.	**57**		**58**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	271.35	$\widehat{\boldsymbol{H1}}$	271.35	$\widehat{\boldsymbol{H9}}$
O_2	1.36	$\widehat{\boldsymbol{H2}}$	1.36	$\widehat{\boldsymbol{H10}}$
N_2	6.87	$\widehat{\boldsymbol{H3}}$	6.87	$\widehat{\boldsymbol{H11}}$
CH_4	117.23	$\widehat{\boldsymbol{H4}}$	117.23	$\widehat{\boldsymbol{H12}}$
CO_2	66.09	$\widehat{\boldsymbol{H5}}$	66.09	$\widehat{\boldsymbol{H13}}$
CO	1.84	$\widehat{\boldsymbol{H6}}$	1.84	$\widehat{\boldsymbol{H14}}$
$H_2O_{(v)}$	196.29	$\widehat{\boldsymbol{H7}}$	196.29	$\widehat{\boldsymbol{H15}}$
$C_{10}H_8$	0.00034	$\widehat{\boldsymbol{H8}}$	0.00034	$\widehat{\boldsymbol{H16}}$
Pressure bar	30		30	
Temperature ^{o}C	721		240	
Reference Temperature ^{o}C	25			

4.16.1.Inlet and outlet enthalpy of WHB-402:

Table 4.47: *Inlet and Outlet Enthalpy of WHB-402.*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H1}}$	20.44
O_2	$\boldsymbol{\widehat{H2}}$	22.58
N_2	$\boldsymbol{\widehat{H3}}$	21.27
CH_4	$\boldsymbol{\widehat{H4}}$	56.73
CO_2	$\boldsymbol{\widehat{H5}}$	39.76
CO	$\boldsymbol{\widehat{H6}}$	21.50
$H_2O_{(v)}$	$\boldsymbol{\widehat{H7}}$	31.21
$C_{10}H_8$	$\boldsymbol{\widehat{H8}}$	104.82

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H9}}$	6.21
O_2	$\boldsymbol{\widehat{H10}}$	7.26
N_2	$\boldsymbol{\widehat{H11}}$	6.32
CH_4	$\boldsymbol{\widehat{H12}}$	13.34
CO_2	$\boldsymbol{\widehat{H13}}$	11.20
CO	$\boldsymbol{\widehat{H14}}$	6.83
$H_2O_{(v)}$	$\boldsymbol{\widehat{H15}}$	9.46
$C_{10}H_8$	$\boldsymbol{\widehat{H16}}$	6.58

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_iH_i)_{prod} - \Sigma(n_iH_i)_{react} \tag{4.22}$$

$$(\boldsymbol{\Delta H})^{\cdot} = \boldsymbol{-15049737.14\ kJ/hr}.$$

Table 4.48: *Utility requirement for WHB-402*

Utility requirement	
As, $\boldsymbol{\dot{Q} = \dot{m} * Cp * \Delta T + \dot{m} * \lambda}$	
Cp at average temperature	4.19 (kJ/kg. ^{0}K)
ΔT	(152-25) ^{0}C
λ at 5 bars	2106.9 kJ/kg
$\boldsymbol{\dot{m}}$	5703 kg/hr.

4.17. Energy balance on methanator (03):

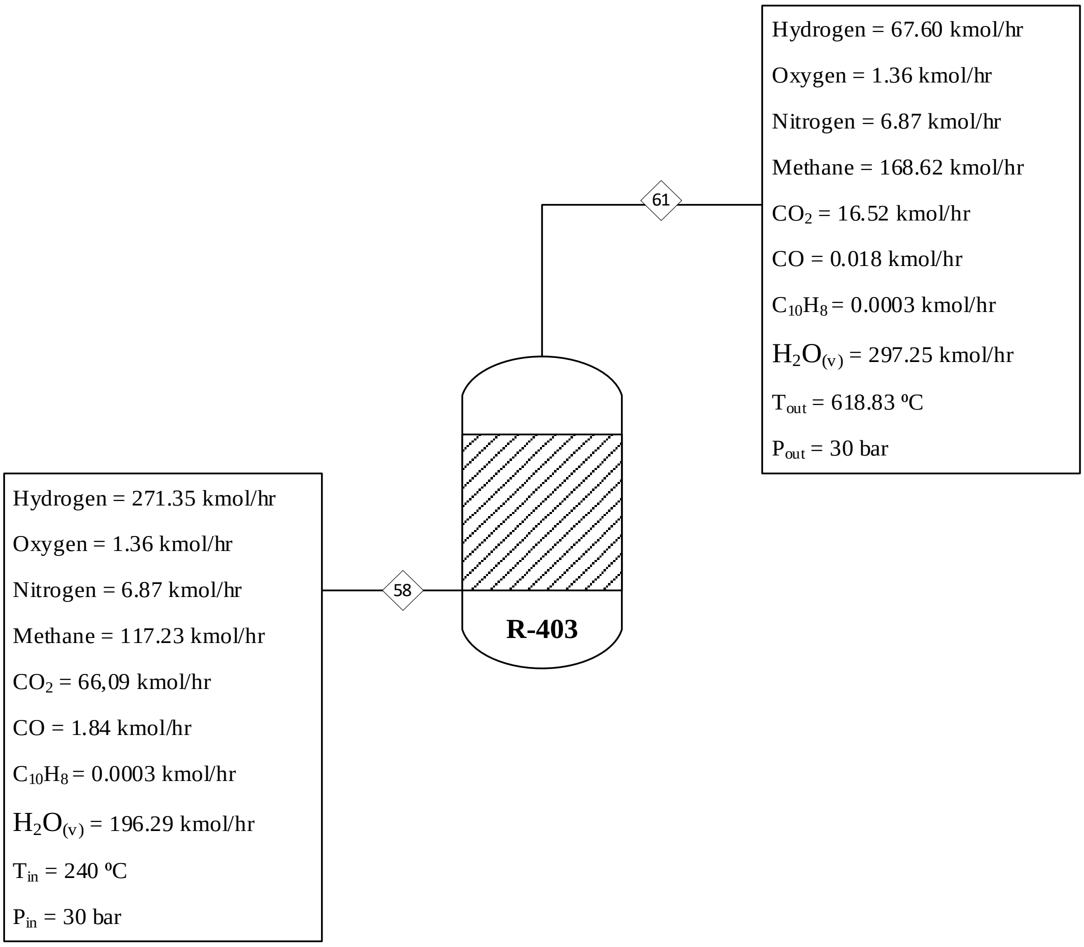

Figure 4.17: *Energy balance on R-403.*

Table 4.49: *Energy balance on methanator-03*

Stream no.	**58**		**61**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	271.35	$\widehat{H1}$	67.60	$\widehat{H9}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H10}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H11}$
CH_4	117.23	$\widehat{H4}$	168.62	$\widehat{H12}$
CO_2	66.09	$\widehat{H5}$	16.52	$\widehat{H13}$
CO	1.84	$\widehat{H6}$	0.018	$\widehat{H14}$
$H_2O_{(v)}$	196.29	$\widehat{H7}$	297.25	$\widehat{H15}$
$C_{10}H_8$	0.00034	$\widehat{H8}$	0.00034	$\widehat{H16}$
Pressure bar	30		30	
Temperature ºC	240		618.83	
Reference Temperature ºC	25			

- The heat of reaction method is applied to solve for adiabatic temperature rise in methanation reactor.

$$\Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\Sigma\varepsilon}^{20} * \Delta H_{ro} \tag{4.23}$$

4.17.1. Inlet and outlet enthalpy of methanator-03

Table 4.50: *Inlet and outlet enthalpy of methanator-03*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H1}}$	6.21
O_2	$\widehat{\boldsymbol{H2}}$	6.55
N_2	$\widehat{\boldsymbol{H3}}$	6.32
CH_4	$\widehat{\boldsymbol{H4}}$	8.94
CO_2	$\widehat{\boldsymbol{H5}}$	8.84
CO	$\widehat{\boldsymbol{H6}}$	6.35
$H_2O_{(v)}$	$\widehat{\boldsymbol{H7}}$	7.42
$C_{10}H_8$	$\widehat{\boldsymbol{H8}}$	6.589

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H9}}$	17.36
O_2	$\widehat{\boldsymbol{H10}}$	19.06
N_2	$\widehat{\boldsymbol{H11}}$	17.98
CH_4	$\widehat{\boldsymbol{H12}}$	30.71
CO_2	$\widehat{\boldsymbol{H13}}$	27.52
CO	$\widehat{\boldsymbol{H14}}$	18.17
$H_2O_{(v)}$	$\widehat{\boldsymbol{H15}}$	21.65
$C_{10}H_8$	$\widehat{\boldsymbol{H16}}$	77.49

$$\boldsymbol{T_{adiabatic} = 618.83\ ^{0}C}$$

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[20] Summation for both reactions

4.18. Energy balance on WHB-403:

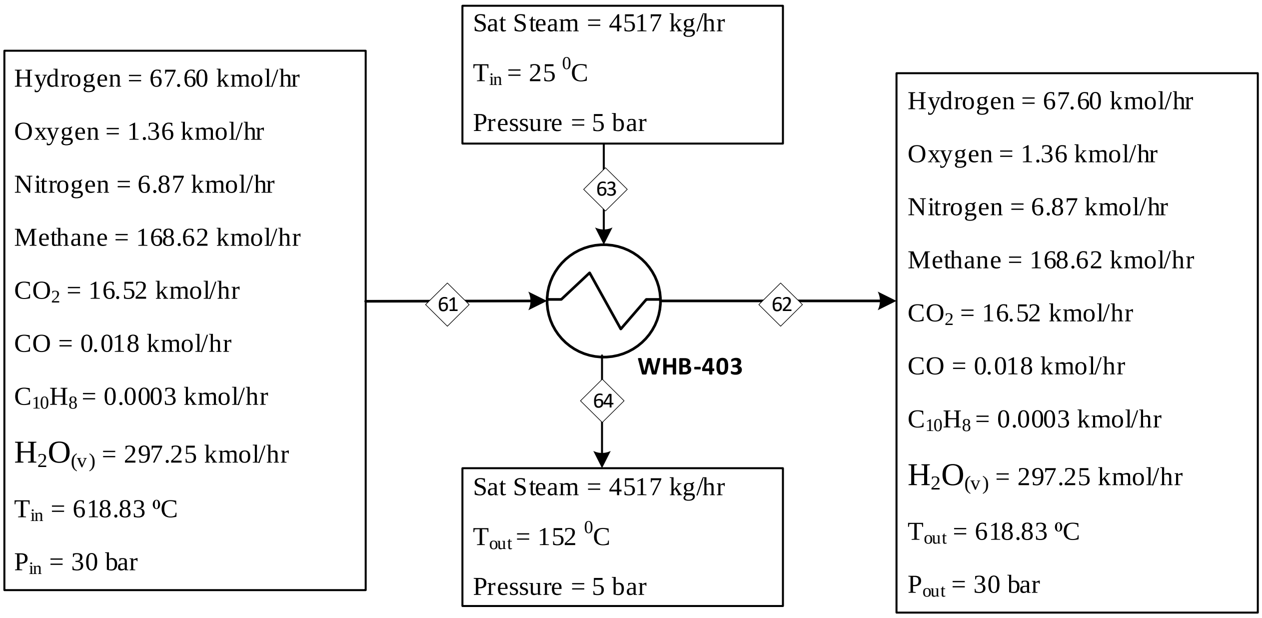


Figure 4.18: *Energy balance on WHB-403.*

Table 4.51: *Energy balance on WHB-403*

Stream no.	**61**		**62**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	67.60	$\widehat{H1}$	67.60	$\widehat{H9}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H10}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H11}$
CH_4	168.62	$\widehat{H4}$	168.62	$\widehat{H12}$
CO_2	16.52	$\widehat{H5}$	16.52	$\widehat{H13}$
CO	0.018	$\widehat{H6}$	0.018	$\widehat{H14}$
$H_2O_{(v)}$	297.25	$\widehat{H7}$	297.25	$\widehat{H15}$
$C_{10}H_8$	0.00034	$\widehat{H8}$	0.00034	$\widehat{H16}$
Pressure bar	30		30	
Temperature ºC	618.8		240	
Reference Temperature ºC	25			

4.18.1.Inlet and outlet enthalpy of WHB-403

Table 4.52: *Inlet and outlet enthalpy of WHB-403*

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H1}}$	17.36
O_2	$\widehat{\boldsymbol{H2}}$	19.06
N_2	$\widehat{\boldsymbol{H3}}$	17.98
CH_4	$\widehat{\boldsymbol{H4}}$	46.51
CO_2	$\widehat{\boldsymbol{H5}}$	33.53
CO	$\widehat{\boldsymbol{H6}}$	18.17
$H_2O_{(v)}$	$\widehat{\boldsymbol{H7}}$	27.25
$C_{10}H_8$	$\widehat{\boldsymbol{H8}}$	77.49

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H9}}$	6.21
O_2	$\widehat{\boldsymbol{H10}}$	7.25
N_2	$\widehat{\boldsymbol{H11}}$	6.32
CH_4	$\widehat{\boldsymbol{H12}}$	13.36
CO_2	$\widehat{\boldsymbol{H13}}$	11.14
CO	$\widehat{\boldsymbol{H14}}$	6.83
$H_2O_{(v)}$	$\widehat{\boldsymbol{H15}}$	9.52
$C_{10}H_8$	$\widehat{\boldsymbol{H16}}$	6.58

$$Total\ Enthalpy\ Change, \Delta H \ = \ \Sigma(n_i H_i)_{prod} \ - \ \Sigma(n_i H_i)_{react} \qquad (4.24)$$

$$(\boldsymbol{\Delta\ H})^{\cdot} \ = \ \boldsymbol{-11927634.15}\ \boldsymbol{kJ/hr}.$$

Table 4.53: *Utility requirement of WHB-403*

Utility requirement	
As, $\dot{\boldsymbol{Q}} = \dot{\mathbf{m}} * \boldsymbol{Cp} * \boldsymbol{\Delta T} + \dot{\mathbf{m}} * \lambda$	
Cp at average temperature	4.19 (kJ/kg. ⁰K)
ΔT	(152-25) ⁰C
λ at 5 bars	2106.9 kJ/kg
$\dot{\boldsymbol{m}}$	4517 kg/hr.

4.19. Energy balance on methanator (04):

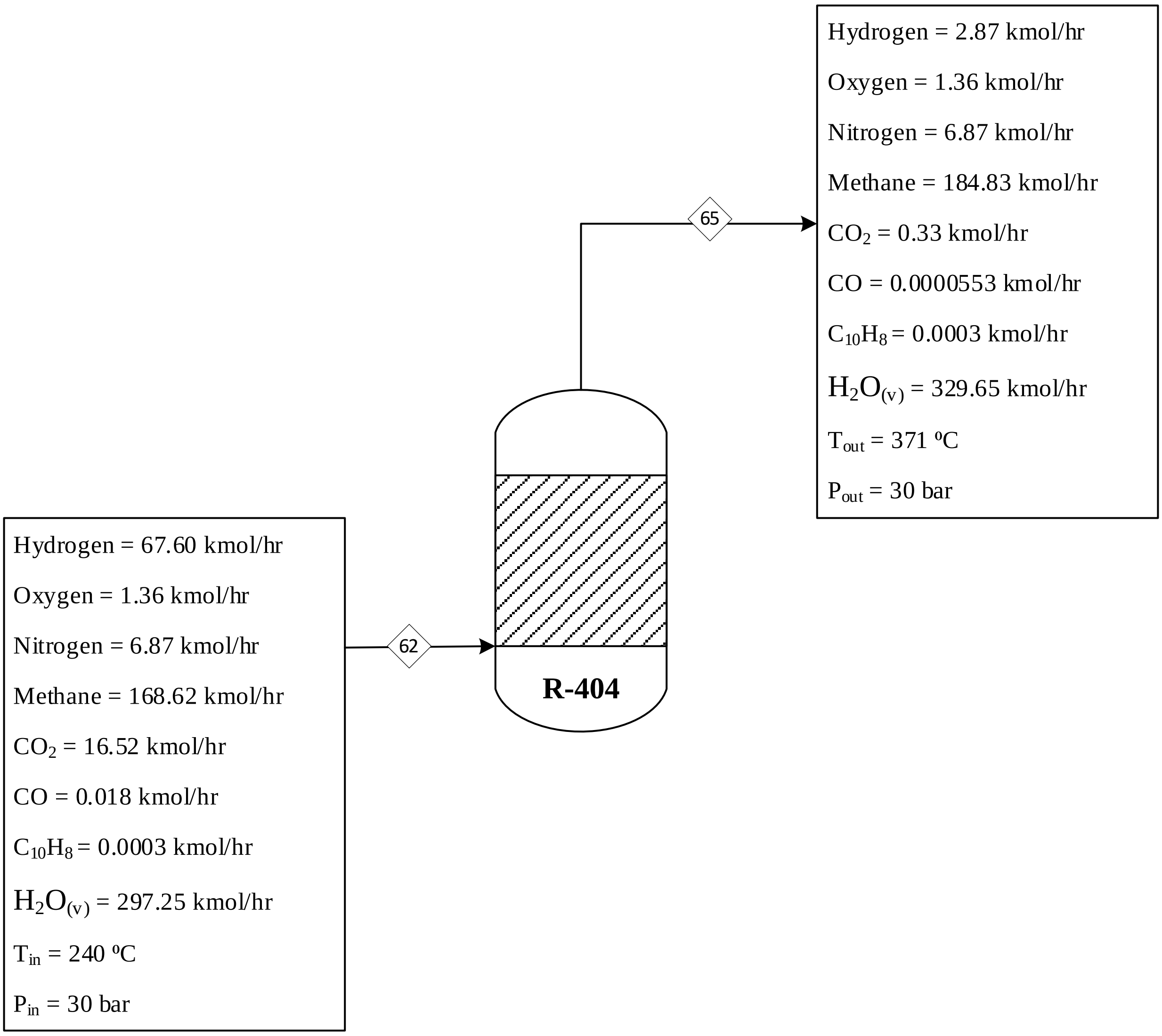


Figure 4.19: *Energy balance on R-404.*

Heat of reaction method was followed to calculate the adiabatic temperature rise in the methanator reactor.

$$Specific\ enthalpy\ changes\ or\ \boldsymbol{\hat{H}} = \int_{\boldsymbol{Tr}}^{\boldsymbol{T}} \boldsymbol{a} + \int_{\boldsymbol{Tr}}^{\boldsymbol{T}} \boldsymbol{bT} + \int_{\boldsymbol{Tr}}^{\boldsymbol{T}} \boldsymbol{cT^2} + \int_{\boldsymbol{Tr}}^{\boldsymbol{T}} \boldsymbol{dT^3} \qquad (4.25)$$

$$Total\ Enthalpy\ Change, \Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\Sigma\varepsilon} * \Delta H_r o \qquad (4.26)$$

- In adiabatic reactor the outlet temperature is normally the desired entity to be found by energy balance. The outlet was found via solving the equation given below,
  $$Total\ Enthalpy\ Change, \Delta H = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react}) + \boldsymbol{\varepsilon} * \Delta H_{ro}$$
- Where $\Delta H = 0$ for adiabatic. The equation becomes,
  $$\boldsymbol{\Sigma\varepsilon} * \Delta H_{ro} = (\Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react})$$

Table 4.54: *Energy balance on methanator-04*

Stream no.	**62**		**65**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	67.60	$\widehat{\boldsymbol{H1}}$	2.78	$\widehat{\boldsymbol{H9}}$
O_2	1.36	$\widehat{\boldsymbol{H2}}$	1.36	$\widehat{\boldsymbol{H10}}$
N_2	6.87	$\widehat{\boldsymbol{H3}}$	6.87	$\widehat{\boldsymbol{H11}}$
CH_4	168.62	$\widehat{\boldsymbol{H4}}$	184.83	$\widehat{\boldsymbol{H12}}$
CO_2	16.52	$\widehat{\boldsymbol{H5}}$	0.33	$\widehat{\boldsymbol{H13}}$
CO	0.018	$\widehat{\boldsymbol{H6}}$	5.52585E-05	$\widehat{\boldsymbol{H14}}$
$H_2O_{(v)}$	297.25	$\widehat{\boldsymbol{H7}}$	329.65	$\widehat{\boldsymbol{H15}}$
$C_{10}H_8$	0.00034	$\widehat{\boldsymbol{H8}}$	0.00034	$\widehat{\boldsymbol{H16}}$
Pressure bar	30		30	
Temperature ^oC	240		371	
Reference Temperature ^oC	25			

4.19.1. Inlet and outlet enthalpy of methanator-04

Table 4.55: *Inlet and outlet enthalpy of methanator-04*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H1}}$	6.21
O_2	$\widehat{\boldsymbol{H2}}$	6.55
N_2	$\widehat{\boldsymbol{H3}}$	6.32
CH_4	$\widehat{\boldsymbol{H4}}$	8.94
CO_2	$\widehat{\boldsymbol{H5}}$	8.84
CO	$\widehat{\boldsymbol{H6}}$	6.35
$H_2O_{(v)}$	$\widehat{\boldsymbol{H7}}$	7.42
$C_{10}H_8$	$\widehat{\boldsymbol{H8}}$	6.58

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\widehat{\boldsymbol{H9}}$	10.02
O_2	$\widehat{\boldsymbol{H10}}$	10.75
N_2	$\widehat{\boldsymbol{H11}}$	10.25
CH_4	$\widehat{\boldsymbol{H12}}$	15.61
CO_2	$\widehat{\boldsymbol{H13}}$	14.9228935
CO	$\widehat{\boldsymbol{H14}}$	10.33
$H_2O_{(v)}$	$\widehat{\boldsymbol{H15}}$	12.14
$C_{10}H_8$	$\widehat{\boldsymbol{H16}}$	24.23

$$Adiabatic\ temperature\ rise, \boldsymbol{T_{ad}} = \mathbf{371}\ {}^{0}\boldsymbol{C}$$

4.20. Energy balance on WHB-404:

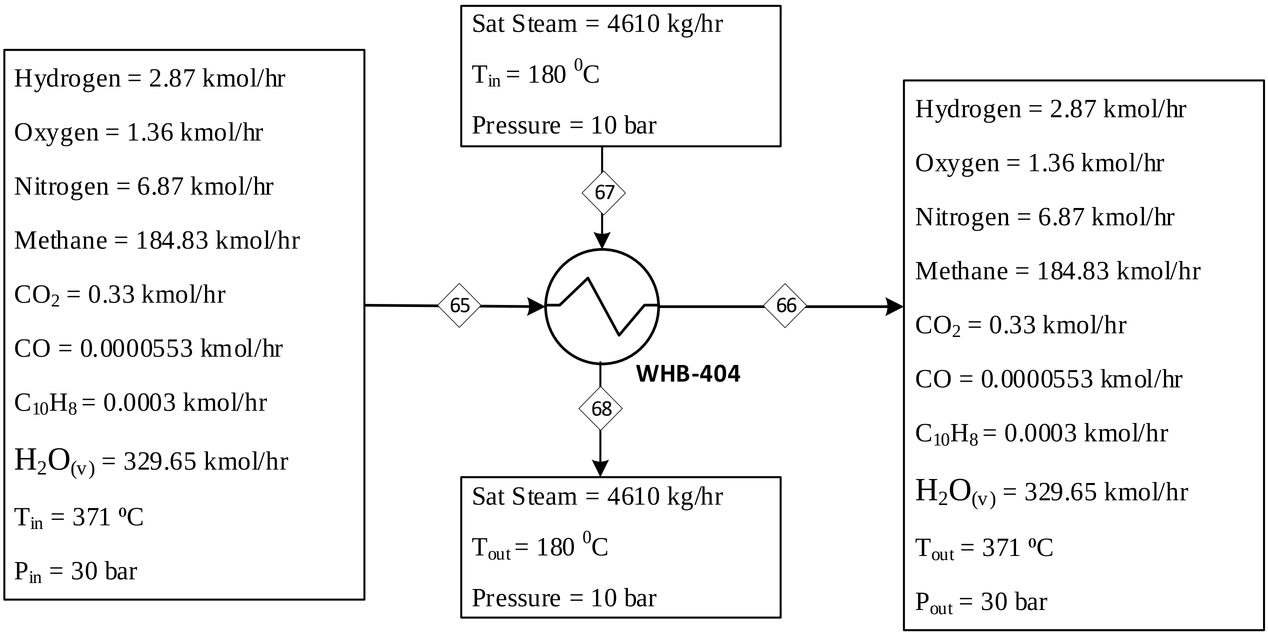


Figure 4.20: *Energy balance on WHB-404.*

Table 4.56: *Energy balance on WHB-404*

Stream no.	**65**		**66**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	2.78	$\widehat{H1}$	2.78	$\widehat{H9}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H10}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H11}$
CH_4	184.83	$\widehat{H4}$	184.83	$\widehat{H12}$
CO_2	0.33	$\widehat{H5}$	0.33	$\widehat{H13}$
CO	5.52585E-05	$\widehat{H6}$	5.52585E-05	$\widehat{H14}$
$H_2O_{(v)}$	329.65	$\widehat{H7}$	329.65	$\widehat{H15}$
$C_{10}H_8$	0.00034	$\widehat{H8}$	0.00034	$\widehat{H16}$
Pressure bar	30		30	
Temperature °C	371		235	
Reference Temperature °C	25			

4.20.1.Inlet and outlet enthalpy of WHB-404

Table 4.57: *Inlet and outlet enthalpy of WHB-404*

Enthalpies of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H1}}$	10.02
O_2	$\boldsymbol{\widehat{H2}}$	10.75
N_2	$\boldsymbol{\widehat{H3}}$	10.25
CH_4	$\boldsymbol{\widehat{H4}}$	23.58
CO_2	$\boldsymbol{\widehat{H5}}$	18.55
CO	$\boldsymbol{\widehat{H6}}$	10.33
$H_2O_{(v)}$	$\boldsymbol{\widehat{H7}}$	14.82
$C_{10}H_8$	$\boldsymbol{\widehat{H8}}$	24.23

Enthalpies of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H9}}$	6.07
O_2	$\boldsymbol{\widehat{H10}}$	7.08
N_2	$\boldsymbol{\widehat{H11}}$	6.17
CH_4	$\boldsymbol{\widehat{H12}}$	13
CO_2	$\boldsymbol{\widehat{H13}}$	10.86
CO	$\boldsymbol{\widehat{H14}}$	6.66
$H_2O_{(v)}$	$\boldsymbol{\widehat{H15}}$	9.29
$C_{10}H_8$	$\boldsymbol{\widehat{H16}}$	6.09

$$Total\ Enthalpy\ Change, \Delta H = \Sigma(n_i H_i)_{prod} - \Sigma(n_i H_i)_{react} \quad (4.27)$$

$$(\boldsymbol{\Delta H})^{\cdot} = \boldsymbol{-3826431.646\ kJ/hr}.$$

Table 4.58: *Utility requirement of WHB-404*

Utility requirement	
As, $\boldsymbol{\dot{Q}} = \dot{\mathbf{m}} * \boldsymbol{Cp} * \boldsymbol{\Delta T} + \dot{\mathbf{m}} * \lambda$	
Cp at average temperature	4.19 (kJ/kg. ⁰K)
ΔT	(152-25) ⁰C
λ at 5 bars	2106.9 kJ/kg
$\boldsymbol{\dot{m}}$	1450 kg/hr.

4.21. Energy balance on partial condenser:

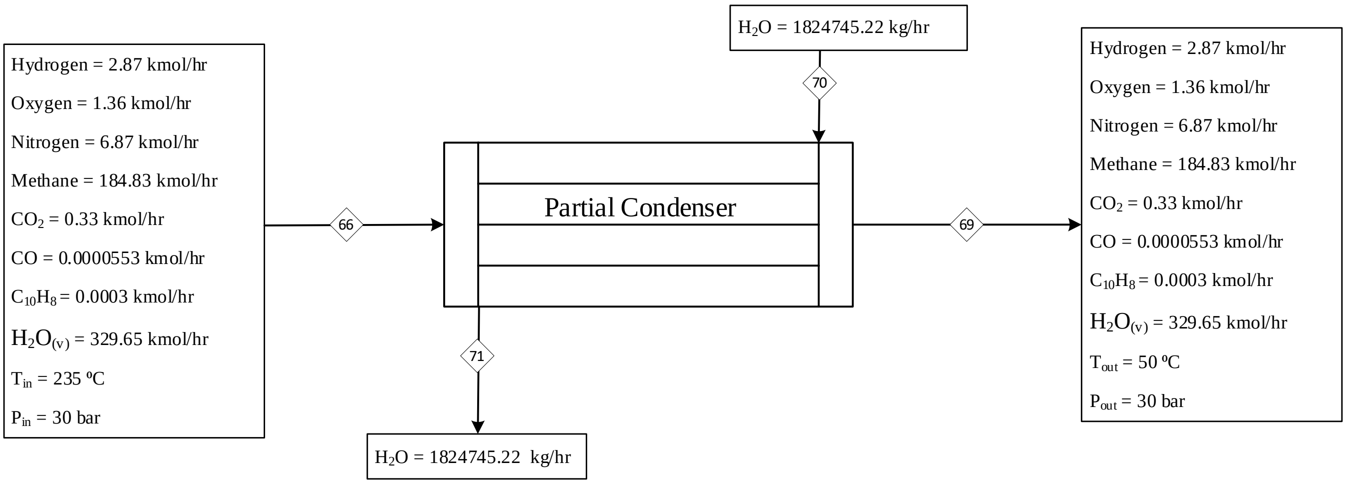


Figure 4.21: *Energy balance on partial condenser (PC-501).*

Table 4.59: *Energy balance on partial condenser*

Stream no.	**66**		**69**	
Stream	**Inlet**		**Outlet**	
Component	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**	**Molar flow (kmol/hr.)**	**Enthalpy (kJ/mol.)**
H_2	2.78	$\widehat{H1}$	2.78	$\widehat{H9}$
O_2	1.36	$\widehat{H2}$	1.36	$\widehat{H10}$
N_2	6.87	$\widehat{H3}$	6.87	$\widehat{H11}$
CH_4	184.83	$\widehat{H4}$	184.83	$\widehat{H12}$
CO_2	0.33	$\widehat{H5}$	0.33	$\widehat{H13}$
CO	5.52585E-05	$\widehat{H6}$	5.52585E-05	$\widehat{H14}$
$H_2O_{(v)}$	329.65	$\widehat{H7}$	329.65	$\widehat{H15}$
$C_{10}H_8$	0.00034	$\widehat{H8}$	0.00034	$\widehat{H16}$
Pressure bar	30		30	
Temperature ºC	235		50	
Reference Temperature ºC	25			

4.21.1. Inlet and outlet enthalpy of partial condenser:

Table 4.60: *Inlet and outlet enthalpy of partial condenser*

Enthalpy of inlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H1}}$	6.07
O_2	$\boldsymbol{\widehat{H2}}$	7.08
N_2	$\boldsymbol{\widehat{H3}}$	6.17
CH_4	$\boldsymbol{\widehat{H4}}$	12.98
CO_2	$\boldsymbol{\widehat{H5}}$	10.90
CO	$\boldsymbol{\widehat{H6}}$	6.66
$H_2O_{(v)}$	$\boldsymbol{\widehat{H7}}$	9.29
$C_{10}H_8$	$\boldsymbol{\widehat{H8}}$	6.09

Enthalpy of outlet stream		
Component	**Enthalpy (kJ/mol.)**	
H_2	$\boldsymbol{\widehat{H9}}$	0.72
O_2	$\boldsymbol{\widehat{H10}}$	0.81
N_2	$\boldsymbol{\widehat{H11}}$	0.72
CH_4	$\boldsymbol{\widehat{H12}}$	1.31
CO_2	$\boldsymbol{\widehat{H13}}$	1.21
CO	$\boldsymbol{\widehat{H14}}$	0.76
$H_2O_{(v)}$	$\boldsymbol{\widehat{H15}}$	-0.94
$C_{10}H_8$	$\boldsymbol{\widehat{H16}}$	-30.24

Table 4.61: *Utility requirement of partial condenser*

Utility requirement	
As, $\dot{Q} = \dot{m} * Cp * \Delta T$	
Average Cp at defined temperature range	1.846 (kJ/kg. ^{o}K)
ΔT	20
$\boldsymbol{\dot{m}}$	182474.22 kg/hr.

CHAPTER # 05

EQUIPMENT DESIGN

5. Equipment design:

5.1. Design of methanator (R-401):

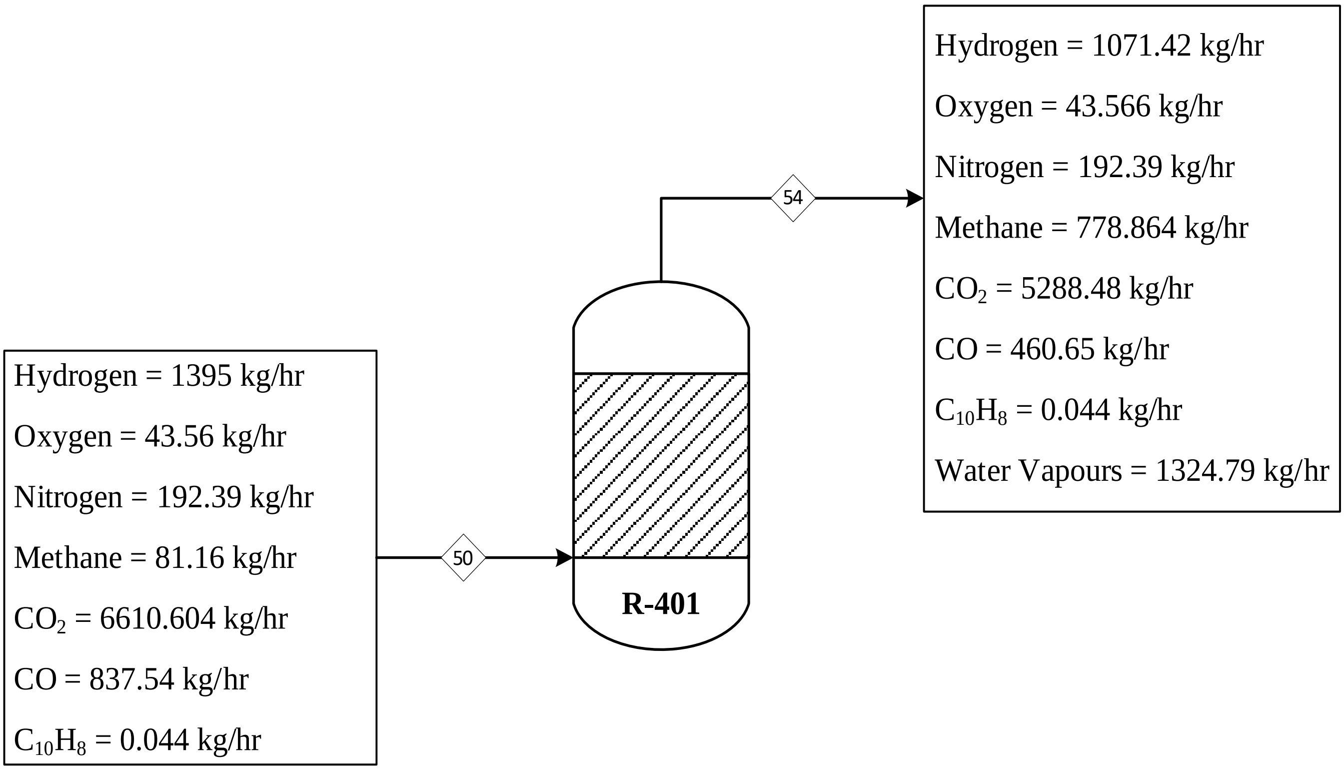


Figure 5.1: *Balance on methanator (R-401)*

5.1.1. Selection of reactor type:

Four selection stages are involved in choosing a reactor model for a specific chemical reaction:

- The reaction will be carried out in one or more stages.
- When there are two or more phases, the reactor structure, or how the phases are arranged in relation to one another, is chosen.
- The mode of operation may be batch or continuous, tubular, or mixed, co-current or countercurrent, and so on.

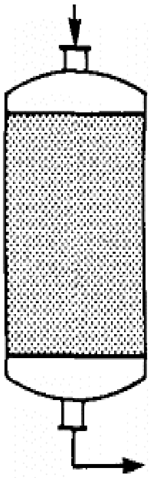
A solid catalyst is used in some catalytic processes that include gas and a liquid. Slurry reactors or three-phase packed beds are often used with them.

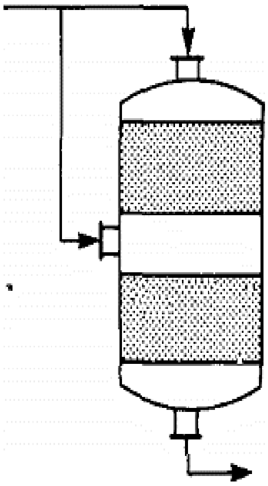
- Fixed-bed reactors are used for solid-catalyzed gas–liquid reactions that are sluggish and necessitate a considerable volume of catalyst compared to slurry reactors.
- Fixed-bed operation has the benefit of keeping the catalyst ions in the reactors and eliminating the need for filtration to isolate them from the oil. This makes continuous operation smoother.
- Since the gas and liquid flows through the reactor are like perfect plug flow, high conversion of one or both reactants are simpler to achieve with a set bed of catalyst.

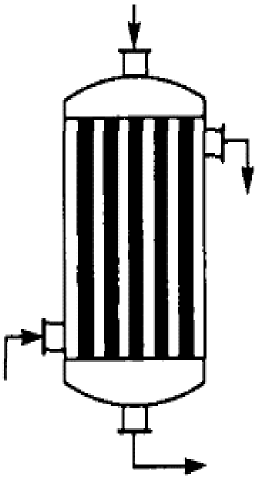
5.1.2. Fixed bed catalytic reactors:

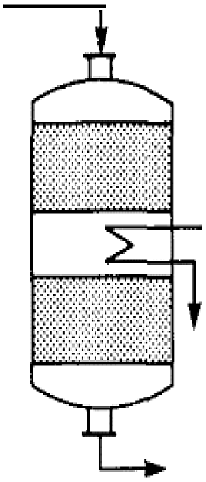
Catalyst particles with a diameter of 2-5 mm are used in fixed beds reactors. A reactor's catalyst can be loaded in a variety of ways, including:

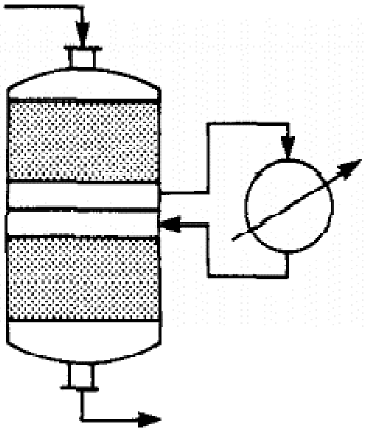
(a) A large single bed.
(b) Several horizontal beds.
(c) A single shell with several filled tubes.
(d) and **(e)** Beds in separate shells.
(f) A single bed of imbedded tubing.

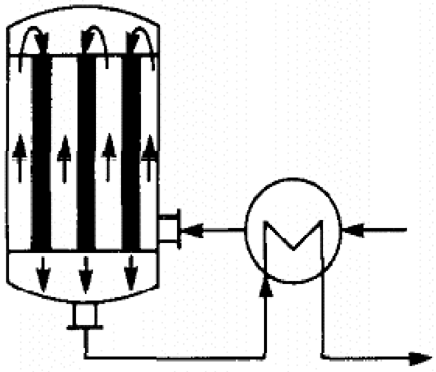

(a)


(b)


(c)


(d)


(e)


(f)

5.1.2.1. Types of fixed bed reactor:

Fixed-bed reactors fall into one of two major categories:

i. Adiabatic

ii. Non-adiabatic.

Several reactor configurations have evolved to fit the unique requirements of specific types of reactions and conditions. Some of the more common ones used for gas-phase reactions are summarized in the table below and the accompanying illustrations. The table can be used for initial selection of a given reaction system, particularly by comparing it with the known systems indicated.

After examining various configurations of fixed bed reactors, we have determined adiabatic fixed bed reactor is the best fit for our system. Since the hydrogenation of carbon oxides is an equilibrium and moderately exothermic reaction, continuous cooling would be required in order to disturb the thermodynamic equilibrium conversion; otherwise, there will be a drastic decrease in rate of reaction which would lead to a huge volume.

Table 5.1: *Selection of fixed-bed reactors*

Classification	Use	Typical Applications
Single adiabatic bed	Moderately exothermic or endothermic non-equilibrium limited	Mild hydrogenation
Radial flow	Where low AP is essential and useful where change in moles is large	Styrene from ethylbenzene
Adiabatic beds in series with intermediate cooling or heating	High conversion, equilibrium limited reactions	-SO2 oxidation -Catalytic reforming -Ammonia synthesis -Hydrocracking Styrene from ethyl benzene
Multi-tabular non-adiabatic	Highly endothermic or Exothermic reactions requiring close temperature control to ensure high selectivity	Many hydrogenations Ethylene-oxidation to Ethylene oxide, formaldehyde by methanol oxidation, phthalic anhydride production
Direct fired. non-adiabatic	Highly endothermic, high temperature reactions	Steam reforming
Single adiabatic bed	Moderately exothermic or endothermic non-equilibrium limited	Mild hydrogenation

5.1.3. Design steps:

1) Solving rate equation for thermodynamically consistent form that consists of conversion as a function of temperature with constant rates.
2) Map out the Levenspiel plot.
3) Weight of Catalyst
4) Volume of Catalyst
5) Volume of Reactor
6) Packing Height
7) Pressure Drop

- **Operating conditions:**

$Temperature\ =\ 350-660\ °C\ (non-isothermal)$

$Pressure\ =\ 30\ bar$

- **Reaction:**

$$CO(g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(v) \qquad (5.1)$$

$$CO_2(g) + 4\,H_2(g) \rightarrow CH_4(g) + 2\,H_2O(v) \qquad (5.2)$$

- **Calculation procedure:**

I. **For Reaction 01:**

$$CO(g) + 3\,H_2(g) \rightarrow CH_4(g) + H_2O(v)$$

Kinetic equation:[53]

$$\boldsymbol{r} = \frac{k_1 * P_{CO} * P_{H_2}{}^{0.5}}{\left(k_2 * P_{H_2}{}^{0.5} + k_3 * P_{CO} + k_4 * P_{H_2O}\right)^2} \tag{5.3}$$

For variable density system,

$Initial\ Volume\ =\ 4\ (Total\ stoichiometric\ moles\ of\ reactant)$
$Final\ Volume\ =\ 2\ (Total\ stoichiometric\ moles\ of\ product)$

$$\varepsilon a = \frac{(Final\ Volume - Initial\ Volume)}{Initial\ Volume} \Rightarrow \frac{(2-4)}{4}$$

$$\boldsymbol{\varepsilon a\ =\ -0.5}$$

Table 5.2: *Terminologies used in fixed bed reactor (methanator).*

Component	**Mass flowrate (kg/hr.)**	**Molar Flowrate (kmol/hr.)**	**Mole Fraction**	**Density (kg/m^3)**	**Volumetric Flowrate[21] (m^3/hr)**
H_2	1395.05	691.99	0.781	0.93	1493.87
O_2	43.56	1.361	0.0015	14.82	2.93
N_2	192.39	6.87	0.0077	12.97	14.83
CH_4	81.16	5.06	0.00571	7.43	10.92
CO_2	6610.60	150.20	0.169	20.38	324.26
CO	837.54	29.90	0.033	12.97	64.55
Sum	9160.39	885.39	1		

- **Volumetric flowrate of mixture:**

$$P\dot{V}\ =\ \dot{n} * RT \tag{5.4}$$

$$\boldsymbol{\dot{V} =\ 1911.39\ (m^3\ /hr)}$$

As, $Fa_o = Ca_o * \dot{\mathbf{V}}$, where Fa_o is initial molar feed rate (kmol/hr).
So, Concentration from the above relation comes out to be,

---

[21] R(m3.bar/K.mol) = 8.31E-05

Table 5.3: *Concentration of components*

Component	Concentration (mol/m^3)
Carbon monoxide (Cco,o)	15.64
Steam (C_{H2O},o)	362.03
Methane (Cch4,o)[22]	7.03
Hydrogen ($C_{H2,o}$)	7.03

$$\varepsilon b = \frac{a*\varepsilon a*C_{bo}}{b*C_{ao}} \tag{5.5}$$

So,

- $\varepsilon b = -3.875$

and

$$X_b = \frac{b*C_{ao}*X_a}{a*C_{bo}} \tag{5.6}$$

- $X_b = 0.129 * X_a$

Due to complexity of rate equation, various attempts were made to transform the kinetic equation in terms of parameters that relates the conversion as a function of temperature. However, another method was devised to get the conversion in its desired form by applying energy balance on non-isothermal (adiabatic) plug flow reactor which relates,

$$X_a = \frac{\sum F_i*Cp_i}{F_{ao}*(-\Delta Hr)} * \Delta T \tag{5.7}$$

Conversion	Initial Temperature (K)	Final Temperature (K)
0	623.15	623.15
0.0997	623.15	643.12
0.1994	643.12	679.56
0.2991	679.56	724.32
0.3988	724.32	767.31
0.4985	767.31	800.47
0.5982	800.47	820.83
0.6979	820.83	830.49
0.7976	830.49	833.84
0.8973	833.84	834.60
0.997	834.60	834.69

---

[22] Product outlet molar flow is found by moles produced from a particular reaction.

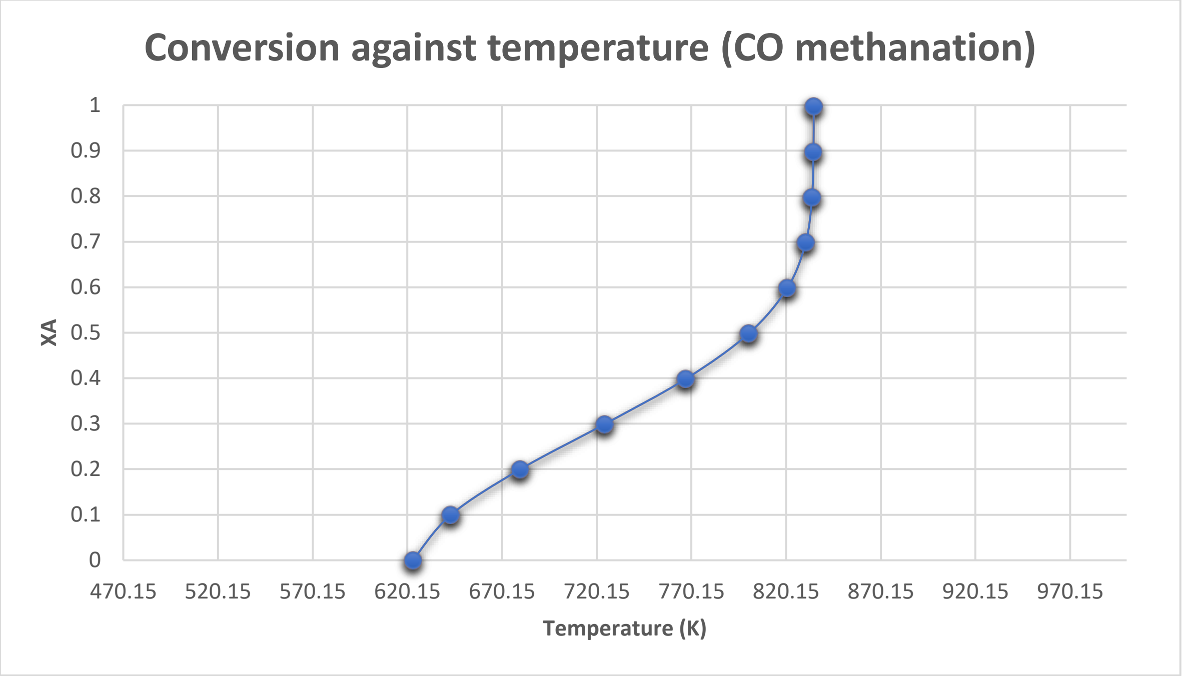


Figure 5.2: *Conversion vs temperature of CO reaction*

1) Weight of catalyst:

$$\frac{\boldsymbol{W}}{\boldsymbol{Fao}} = \int_{\mathbf{0}}^{\boldsymbol{Xa}} \frac{\boldsymbol{dXa}}{(\boldsymbol{-ra})} \qquad (5.8)$$

To draw the lewenspiel plot, convert the kinetic equation into form that consists of rate as function of conversion. So, after mathematical manipulation,

$$r = \frac{6000\, exp\left(\frac{-2483}{T}\right)*\left(1.36T*\frac{1-Xa}{1-0.5Xa}\right)*\left(30.381T*\left(\frac{1-0.129Xa}{1-0.5Xa}\right)\right)^{0.5}}{\left[0.063\, exp\left(\frac{-1505}{T}\right)*\left(30.381T*\left(\frac{1-0.129Xa}{1-0.5Xa}\right)\right)^{0.5}+0.02\, exp\left(\frac{3018}{T}\right)*\left(1.36T*\frac{1-Xa}{1-0.5Xa}\right)*8.67E-18\, exp\left(\frac{19627}{T}\right)*C_{H_2O}*0.08314*T\right]} \qquad (5.9)$$

Were,

- $k1 = 60000EXP(\frac{-2483}{T})$
- $k2 = 0.063EXP(\frac{1505}{T})$
- $k3 = 0.02EXP(\frac{3018}{T})$
- $k4 = 8.67E - 18EXP(\frac{19627}{T})$

It should be contemplated that the simplified rate consists of two variables namely T and Xa ($\boldsymbol{C_{H_2O}}$can be found via $F\boldsymbol{H_2O}$ / V_o) and the rate constants consist of variable T (not a fixed temperature). By applying Simpson’s Quadrature formula for first Methanator (1),

$$\int_{\boldsymbol{Xo}}^{\boldsymbol{X4}} \boldsymbol{f(X)dX} = \frac{\boldsymbol{h}}{\mathbf{3}} * (\boldsymbol{f(xo)} + \mathbf{4}\boldsymbol{f(x1)} + \mathbf{2}\boldsymbol{f(x2)} + \mathbf{4}\boldsymbol{f(x3)} + \boldsymbol{f(x4)}) \qquad (5.10)$$

***Table 5.4:** Solving rate reaction of fixed bed reactor.*

Xa	T(K)	(-ra)[23]	1/(-ra)
0	623.15	26.72	0.037
0.1125	647.4	46.83	0.021
0.225	691.2	112.23	0.008
0.3375	741.2	270.73	0.0036
0.45	784.7	551.86	0.0018

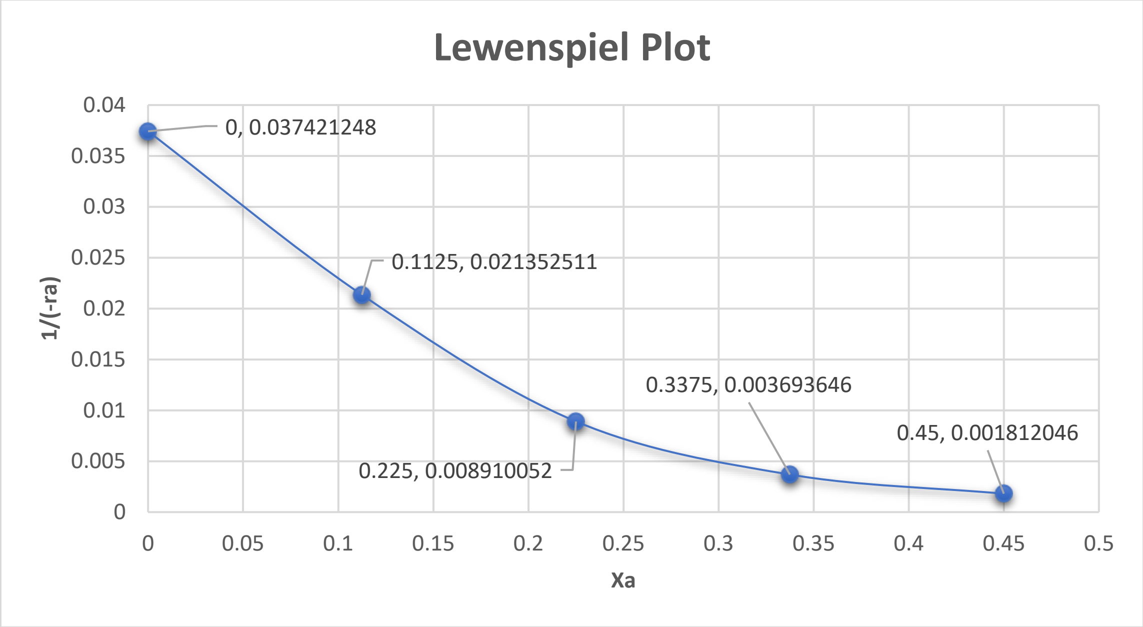


***Figure 5.3:** Levenspiel plot of reaction 1*

It can be noticed from the Levenspiel plot, that with increasing temperature the rate of reaction increases for reversible exothermic reactions as mentioned in general graphical design procedures for non-isothermal reactors. So,

$$Weight\ of\ Catalyst\ (kg)\ =\ ((Area\ under\ the\ curve)\ *(Fao)*1E6))/1000$$

$$=\ ((0.00589)\ *(29.9)\ *(1E6))/1000$$

$$\boldsymbol{Weight\ of\ Catalyst\ =\ 176.31\ kg}$$

$Catalyst\ Used$: $\boldsymbol{MCR-2X}$

II. For reaction 02:

$$CO_2(g)\ +\ 4H_2(g)\ \rightarrow\ CH_4(g)\ +\ 2H_2O(v)$$

Kinetic equation:

$$(-\boldsymbol{rco2}) = \frac{(K_{ch_4} * K_h{}' * K_h * K_a * K_a{}' * KCO_2)^{\frac{1}{3}} * P_{H_2} * P_{CO_2}{}^{\frac{1}{3}}}{1 + K_{CO_2} * P_{CO_2} + K_{H_2} * P_{H_2}} \quad (5.11)$$

Where,

- $K_{ch_4}\ (mmol/gr.sec.atm)\ =\ 8.18$
- $K_h'\ (mmol/gr.sec.atm)\ =\ 0.27$
- $K_h\ (mmol/gr.sec.atm)\ =\ 0.14$
- $K_a\ (mmol/gr.sec)\ =\ 0.41$

---

[23] Units of rate are (mmol/g_{cat}.hr)

- $K'_a = 0.013$
- $K_{co_2}\,(atm) - 1 = 0.028$
- $K_{h2}\,(atm) - 1 = 0.69$

Table 5.5: *Concentration of reaction 2*

Component	Concentration (mol/m^3)
Carbon Dioxide ($C_{co2,o}$)	78.58507624
Steam ($C_{H2O,o}$)	362.0365779
Methane (Cch4,o)[24]	15.71701525
Hydrogen ($C_{H2,o}$)	31.4340305

Now from the same equation used above for parametrizing conversion as a function of temperature, a same plot was plotted for reaction 02.

$$\boldsymbol{Xa} = \frac{\sum \boldsymbol{Fi}*\boldsymbol{Cpi}}{\boldsymbol{Fao}*(-\Delta \boldsymbol{Hr})} * \Delta \boldsymbol{T} \qquad (5.12)$$

Conversion	Initial Temperature (K)	Final Temperature (K)
0	623.15	623.15
0.098	623.15	702.79
0.196	702.79	861.21
0.294	861.21	1092.61
0.392	1092.61	1382.18
0.49	1382.18	1698.47
0.588	1698.47	1986.12
0.686	1986.12	2181.73
0.784	2181.73	2269.12
0.882	2269.12	2292.37
0.98	2292.37	2295.49

---

[24] Product outlet molar flow is found by moles produced from a particular reaction.

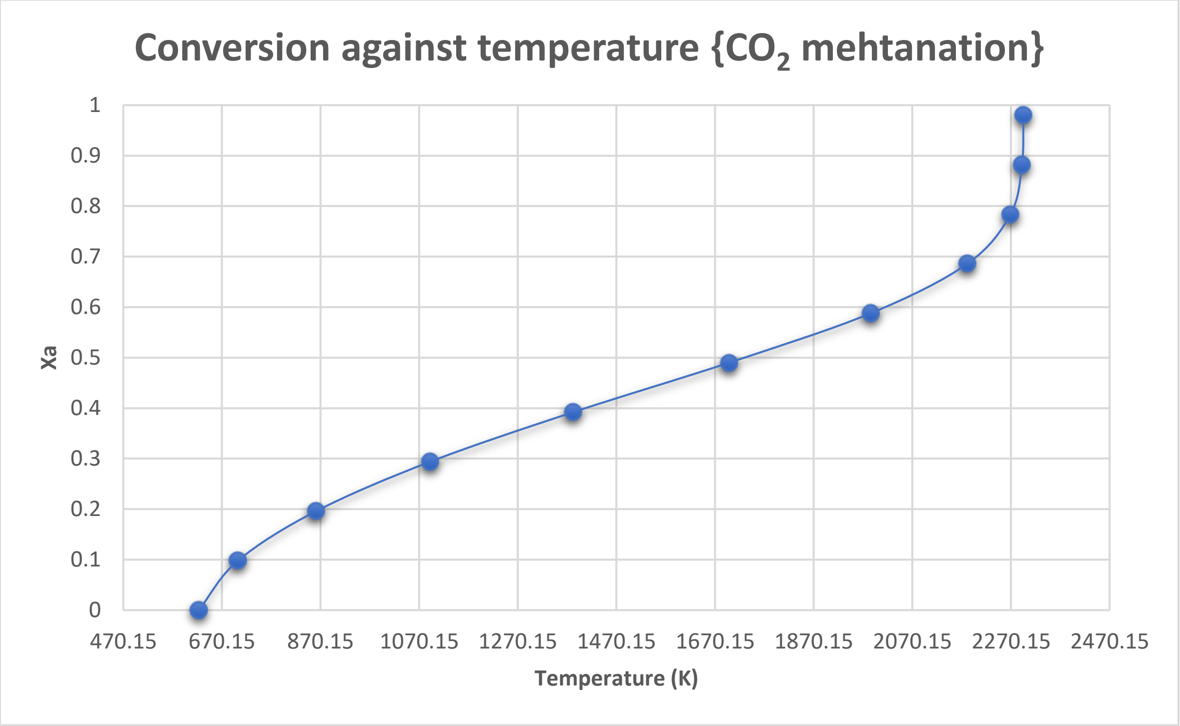


Figure 5.4: *Conversion vs temperature of CO_2 reaction*

$$\boldsymbol{\varepsilon a = -0.4}$$
$$\boldsymbol{\varepsilon b = -0.4625}$$
$$\boldsymbol{X_b = 0.868 * Xa}$$

- **Weight of catalyst:**

$$\frac{W}{F_{ao}} = \int_0^{Xa} \frac{dX_a}{(-r_a)} \tag{5.13}$$

Lewenspiel plot is drawn from following manipulated equation,

$$(-rco_2) = \frac{\left(K_{ch4}*K_h{}'*K_h*K_a*K_a{}'*K_{CO_2}\right)^{\frac{1}{3}}*\left(8.29E-3T*\left(\frac{1-0.864Xa}{1-0.399Xa}\right)\right)*\left(1.7931E-3T*\left(\frac{1-Xa}{1-0.4Xa}\right)\right)^{\frac{1}{3}}}{1+K_{CO_2}\left(1.793-3T*\left(\frac{1-Xa}{1-0.4Xa}\right)\right)+KH2*\left(8.29E-3T*\left(\frac{1-0.864Xa}{1-0.399Xa}\right)\right)} \tag{5.14}$$

$By\ applying\ Simpson's\ Quadrature\ formula\ for\ first\ Methanator\ (1),$

Table 5.6: *Solving rate reaction of reaction 2*

Xa	T(K)	(-ra)[25]	1/(-ra)
0	623.15	0.076	13.15
0.05	664	0.077	12.97
0.1	706.27	0.077	12.82
0.15	787.37	0.080	12.45
0.2	871.46	0.082	12.142

---

[25] Units of rate are (mmmol/g_{cat}.sec)

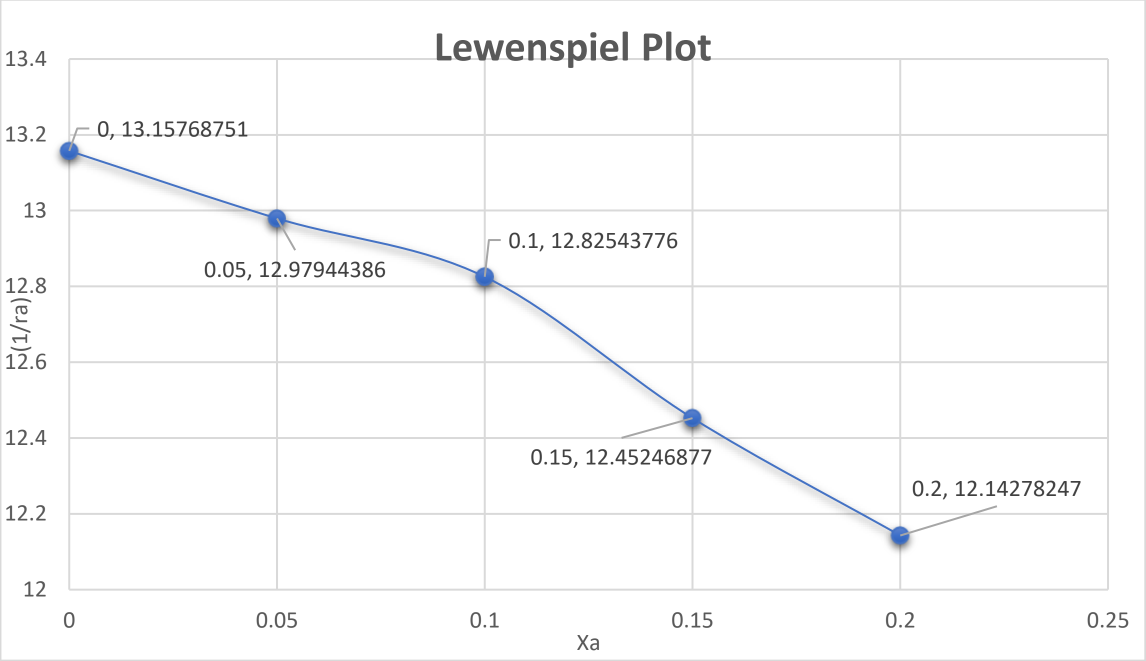


Figure 5.5: *Levenspiel plot of reaction 2*

Again, it should be observed that with increasing temperature, the rate of reaction increases.

$$Weight\ of\ Catalyst\ (g)\ =\ ((Area\ under\ the\ curve)\ *(F_{ao})*1E6)/3600$$

$$=\ ((2.544)\ *(150)\ *(1E6))/3600$$

$$=\ 106173.3133\ g$$

$$\boldsymbol{Weight\ of\ Catalyst\ =\ 106.173\ kg}$$

$Total\ Weight\ of\ Catalyst$: $\boldsymbol{282.486\ kg}$

2) Volume of catalyst:

$$Volume\ of\ Catalyst = \frac{Weight\ of\ Catalyst}{Bulk\ Density\ of\ Catalyst^{26}}$$

$$\boldsymbol{Volume\ of\ Catalyst\ =\ 0.86\ m^3}$$

3) Volume of reactor:

$$Volume\ of\ Reactor\ =\ Volume\ of\ Catalyst\ +\ Void\ Volume$$

$Void\ Volume\ =\ 3.5\ (cm^3/gcat)$

$Void\ Volume\ =\ 0.98\ (m^3)$

$$\boldsymbol{Volume\ of\ Reactor} =\ \mathbf{1.85}\ m^3$$

As, space time is given by,

$$\tau\ =\ (\frac{V}{\dot{V}})$$

$$\boldsymbol{\tau\ =\ 3.5\ sec}$$

4) Height of the shell:

Let

- H/D[27] ratio be 40.
- Diameter of particles dp is 5 mm.

As,

---

[26] Bulk Density of Catalyst = 325 (kg/m^3)

[27] For PBR H/D ratio ranges from 20 to 40

$$V = \pi * \left(\frac{D^2}{4}\right) H \tag{5.15}$$

So, replacing H = 40D we get,

$$D = 0.38\, m$$
$$H = 15.5\, m$$

$Safety\ Holdup\ for\ TOP = 10\%$
$Safety\ Holdup\ for\ BOTTOM = 10\%$

- $Total\ height\ of\ Shell = 18.7\ m$
- $Area\ of\ Reactor = 0.119\ m2$
- $Height\ of\ packing$[28] $= 7.29\ m$

5) Pressure drop[29]:

$$\boldsymbol{\Delta P = [\frac{150*\mu*(1-\varepsilon)*uo}{\varepsilon^3*Dp^2*\varphi^2} + \frac{1.75*\rho f*(uo)^2}{\varepsilon^3*Dp*\varphi}]} \tag{5.16}$$

Where,

- $\boldsymbol{\varepsilon} = Porosity$
- $\boldsymbol{\mu_m} = Gaseous\ mixture\ Viscosity\ (Pa.s)$

$$\mu_m = \frac{\sum_1^n yi*\mu i*(\sqrt{MW})}{\sum_1^n (yi*\sqrt{MW})} \tag{5.17}$$

- $Dp = Diameter\ of\ particle\ (m)$
- $\boldsymbol{\rho f} = Fluid\ Density\ (kg/m3)$
- $\boldsymbol{uo} = Superficial\ Velocity$[30] $(m.s)$

$$\Delta P = \left[\frac{150 * 2.167E - 5 * (1 - 0.58) * 4.454}{0.58^3 * 0.005^2 * 0.58^2} + \frac{1.75 * 4.73 * (4.45)^2}{0.58^3 * 0.005 * 0.58}\right]$$

$$\Delta P = 294210.59\ Pa$$
$$\boldsymbol{\Delta P = 2.94\ bar}$$

---

[28] Vcat = $\pi * r * Lcat$
[29] From Unit Operations of Chemical Engineering by Warren L. McCabe
[30] Superficial Velocity = (Volumetric Flowrate/Area)

Table 5.7: *Specification of methanator-01*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	$R-401$
Operation	Continuous
Type	Adiabatic packed bed reactor
Function	
Hydrogenation of carbon oxides to methane	
Chemical reaction:	
$CO(g) + 3H2(g) \rightarrow CH4(g) + H2O(v)$ $CO2(g) + 4H2(g) \rightarrow CH4(g) + 2H2O(v)$	
Catalyst	$MCR-2X$ Size $= 5\ mm$ Weight of Catalyst $= 285\ kg$
Diameter of reactor	$0.4\ m$
Volume of reactor	$2\ m^3$
Space time	$4\ sec$
Packing height	$7.3\ m$
Height of reactor	$19\ m$
Area of reactor	$0.12\ m^2$
Pressure drop	$2.9\ bar$

Table 5.8: *Specification sheet of methanator-2*

$Design\ of\ methanator\ (R-402)$

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	$R-402$
Operation	Continuous
Type	Adiabatic packed bed reactor
Function	
Hydrogenation of carbon oxides to methane	
Chemical reaction:	
$CO(g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(v)$ $CO_2(g) + 4H_2(g) \rightarrow CH_4(g) + 2H_2O(v)$	
Catalyst	$MCR-2X$ $Size = 5mm$ $Weight\ of\ Catalyst = 256\ kg$
Diameter of reactor	$0.38\ m$
Volume of reactor	$1.7\ m^3$
Space time	$4\ sec$
Packing height	$7\ m$
Height of reactor	$18\ m$
Area of reactor	$0.11\ m^2$
Pressure drop	$3\ bars$

Table 5.9: *Specification sheet of methanator-3*

$Design\ of\ methanator\ (R-403)$

SPECIFICATION SHEET	
Identification	
$Item$	$Reactor$
$Item\ no.$	$R-403$
$Operation$	$Continuous$
$Type$	$Adiabatic\ packed\ bed\ reactor$
Function	
$Hydrogenation\ of\ carbon\ oxides\ to\ methane$	
$Chemical\ reaction$:	
$CO(g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(v)$ $CO_2(g) + 4H_2(g) \rightarrow CH_4(g) + 2H_2O(v)$	
$Catalyst$	$MCR-2X$ $Size = 5mm$ $Weight\ of\ Catalyst = 194\ kg$
$Diameter\ of\ reactor$	$0.35\ m$
$Volume\ of\ reactor$	$1.3\ m^3$
$Space\ time$	$4\ sec$
$Packing\ height$	$6\ m$
$Height\ of\ reactor$	$17\ m$
$Area\ of\ reactor$	$0.09\ m^2$
$Pressure\ drop$	$3\ bars$

Table 5.10: *Specification sheet of methanator-4*

Design of methanator ($R - 404$)

SPECIFICATION SHEET	
Identification	
Item	*Reactor*
Item no.	$R - 404$
Operation	*Continuous*
Type	*Adiabatic packed bed reactor*
Function	
Hydrogenation of carbon oxides to methane	
Chemical reaction:	
$CO(g) + 3H_2(g) \rightarrow CH_4(g) + H_2O(v)$ $CO_2(g) + 4H_2(g) \rightarrow CH_4(g) + 2H_2O(v)$	
Catalyst	$MCR - 2X$ *Size* = 5.5 *mm* *Weight of Catalyst* = 132 *kg*
Diameter of reactor	0.3 *m*
Volume of reactor	0.86 m^3
Space time	3 *sec*
Packing height	5 *m*
Height of reactor	15 *m*
Area of reactor	0.07 m^2
Pressure drop	2.94 *bars*

5.2. Design of water gas shift reactor (R-301):

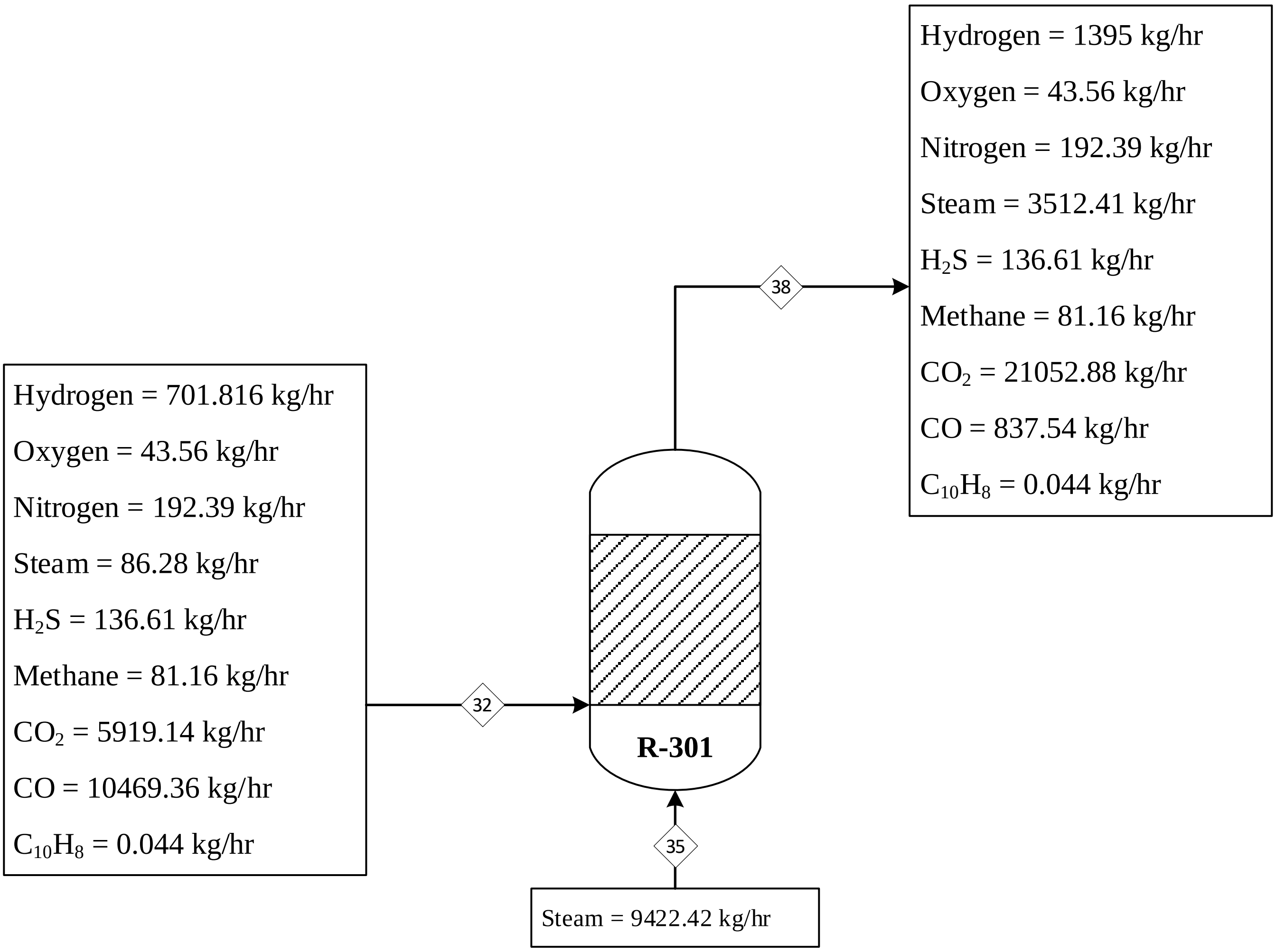


***Figure 5.6:** Balance on WGS unit*

5.2.1. Design steps:

1) Weight of Catalyst
2) Volume of Catalyst
3) Volume of Reactor
4) Number of Tubes
5) Diameter of Reactor
6) Height of Reactor
7) Pressure Drop

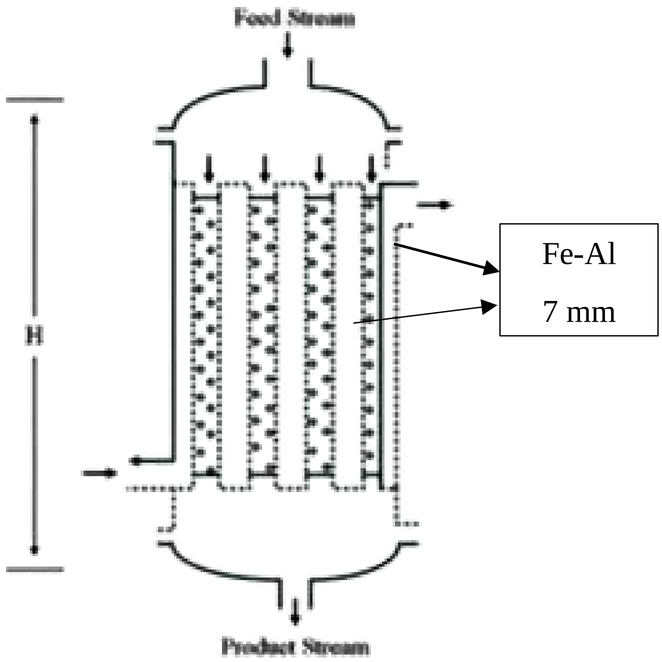


Figure 5.7: *Water gas shift reactor (R-301)*

- ***Operating conditions***:

$Temperature\ =\ 350\,°C$

$Pressure\ =\ 5\ bar$

- ***Reaction***:

$$CO(g)\ +\ H_2O(v)\ \rightarrow\ CO_2(g)\ +\ H_2(g)$$

- ***Calculation procedure***:

Performance equation of PBR:

$$\frac{\boldsymbol{W}}{\boldsymbol{Fao}} = \int_{\boldsymbol{0}}^{\boldsymbol{Xa}} \frac{\boldsymbol{dXa}}{(-\boldsymbol{ra})} \tag{5.18}$$

Kinetic equation: [54]

$$r_{co} = 2.96E5 * Exp\left(\frac{-47400}{RT}\right) * \left(Pco * PH2O - \frac{Pco2*PH2}{Ke}\right) \tag{5.19}$$

For Variable Density System,

$Initial\ Volume\ =\ 2\ (Total\ stoichiometric\ moles\ of\ reactant)$

$Final\ Volume\ =\ 2\ (Total\ stoichiometric\ moles\ of\ product)$

$$\varepsilon = \frac{(\boldsymbol{Final\ Volume} - \boldsymbol{Initial\ Volume})}{\boldsymbol{Initial\ Volume}} \Rightarrow \frac{(\boldsymbol{2}-\boldsymbol{2})}{\boldsymbol{2}}$$

$$\boldsymbol{\varepsilon\ =\ 0}$$

Table 5.11: *Terminologies used in water gas shift reactor.*

Component	Mass Flowrate (kg/hr.)	Molar Flowrate (kmol/hr.)	Mole Fraction	Density (g/m^3)	Volumetric Flowrate[31] (m^3/hr.)
H2	701.81	348.12	0.24	194.56	3607.16
O2	43.56	1.36	0.00096	3088.28	14.10
N2	192.39	6.87	0.0048	2702.24	71.19
H2S	136.61	4.01	0.002	3290.95	41.51
CH4	81.16	5.06	0.0035	1548	52.43
CO2	5919.14	134.50	0.09	4247.35	1393.60
CO	10469.36	373.77	0.26	2703.21	3872.93
H_2O	9707.23	538.84	0.38	1738.60	5583.34
$C_{10}H_8$	0.0443	0.000346	2.44838E-07	12369.54	0.0035
Total	27251.35	1412.53	1		

- $\boldsymbol{Density\ of\ gaseous\ mixture}$:

$$\rho_m = \frac{\sum_1^n \rho_i * \dot{V}_i}{\sum_1^n \dot{V}_i} \tag{5.20}$$

- $\boldsymbol{Volumetric\ flowrate\ of\ mixture}$:

$$\dot{V} = \frac{\dot{m}}{\rho_i} \tag{5.21}$$

$$\boldsymbol{\dot{V} = 14633.29\ (m^3/hr)}$$

$As, F_{ao} = C_{ao} * \dot{\boldsymbol{V}}, where\ F_{ao}\ is\ initial\ molar\ feed\ rate\ (kmol/hr).$
$So, Concentration\ from\ the\ above\ relation\ comes\ out\ to\ be,$

Table 5.12: *Concentration of component used in WGS reactor*

Component	Concentration (mol/m^3)
Carbon monoxide (Cco,o)	25.53
Steam (C_{H2O},o)	36.81
Carbon Dioxide (Cco$_2$,o)[32]	23.49
Hydrogen ($C_{H2,o}$)	23.49

---

[31] R(m3.bar/K.mol) = 8.31E-05

[32] Product outlet molar flow is found by moles produced from a particular reaction

1) $\boldsymbol{Weight\ of\ catalyst}$:

$$\frac{W}{Fao} = \int_{0}^{Xa} \frac{dXa}{(-ra)} \tag{5.22}$$

To draw the Levenspiel plot, convert the kinetic equation into form that consists of rate as function of conversion. So,

$$r_{co} = 31.47 * (1.30 * (1 - X_a) * 0.051 * (36.81 - 25.53 * X_a) - 0.076 \tag{5.23}$$

By applying Simpson's Quadrature formula i.e.,

$$\int_{\boldsymbol{Xo}}^{\boldsymbol{X4}} \boldsymbol{f}(\boldsymbol{X})\boldsymbol{dX} = \frac{\boldsymbol{h}}{\boldsymbol{3}} * (\boldsymbol{f}(\boldsymbol{xo}) + \boldsymbol{4f}(\boldsymbol{x1}) + \boldsymbol{2f}(\boldsymbol{x2}) + \boldsymbol{4f}(\boldsymbol{x3}) + \boldsymbol{f}(\boldsymbol{x4})) \tag{5.24}$$

Table 5.13: *Solving rate equation of WGS reactor*

Xa	**(-ra)**[33]	**1/(-ra)**
0	75.03	0.013
0.23	47.77	0.020
0.46	26.18	0.038
0.69	10.26	0.097
0.92	0.014	69.37

$$Weight\ of\ Catalyst\ (g) = (Area\ under\ the\ curve) * (F_{ao}) * 1000 = (5.36) * (373.77) * (1000)$$

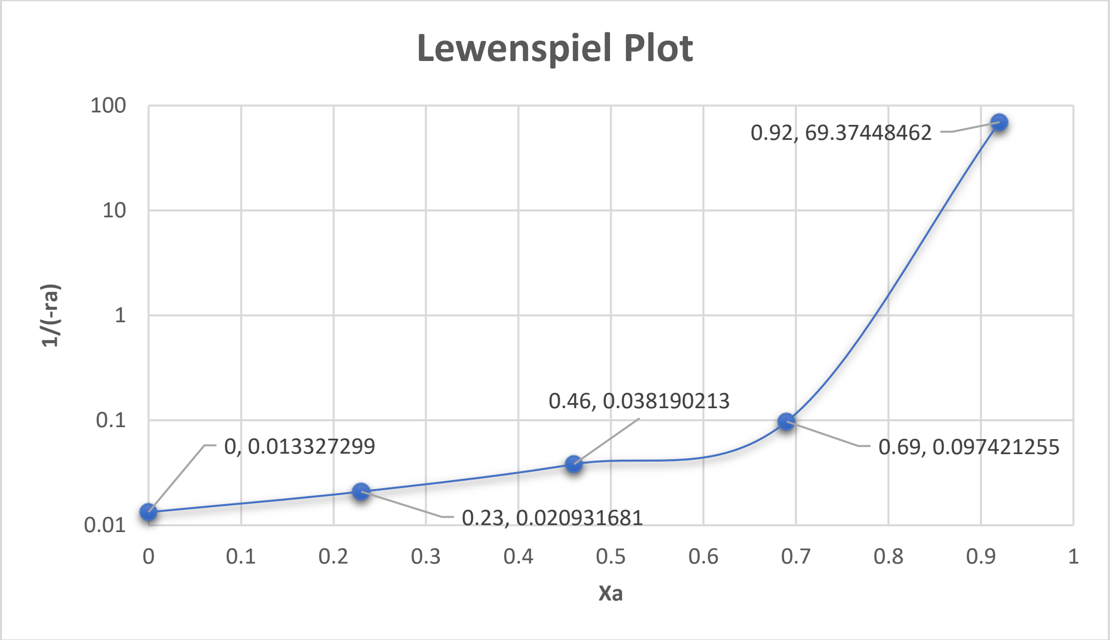


Figure 5.8: *Levenspiel plot of WGS reactor*

$$\boldsymbol{Weight\ of\ catalyst\ =\ 2004.12\ kg}$$

$Catalyst\ Used$: $\boldsymbol{Iron - Aluminum\ (Fe - Al)}$

2) $\boldsymbol{Volume\ of\ catalyst}$:

---

[33] Units of rate are (mol/g_{cat}.hr)

$$Volume\ of\ Catalyst = \frac{Weight\ of\ Catalyst}{Bulk\ Density\ of\ Catalyst^{34}}$$

$$\boldsymbol{Volume\ of\ Catalyst\ =\ 1.56\ m^3}$$

3) *Volume of reactor*:

$$Volume\ of\ Reactor = Volume\ of\ Catalyst + Void\ Volume$$

$\boldsymbol{\epsilon = 0.58}$

$$Volume\ of\ reactor = \frac{Volume\ of\ catalyst}{1 - \epsilon}$$

$$\boldsymbol{Volume\ of\ Reactor =\ 3.67}\ \mathrm{m}^3$$

As, space time is given by,

$$\tau\ =\ (\frac{\boldsymbol{V}}{\dot{\boldsymbol{V}}})$$

$$\tau\ =\ 0.90\ sec$$

4) *Number of Tubes*:

Let,

The nominal length of tubes be 16*ft*.

$$Dia\ of\ tube\ Dt\ be\ 15\ cm\ (should\ be\ between\ (8 - 15)\ cm\ due\ to\ accepted\ heuristics\ for\ plug\ flow\ in\ tubular\ reactor)$$

Diameter of particles dp be 7*mm*.

So,

$$\frac{\boldsymbol{Dt}}{\boldsymbol{dp}} = \frac{\boldsymbol{14 * 10}}{\boldsymbol{7}} = \boldsymbol{21.4 \gg 15}\ (To\ avoid\ deviation\ from\ plug\ flow)$$

$$Volume\ of\ one\ tube\ =\ \boldsymbol{\pi * r^2 * L}$$

$$Volume\ of\ one\ tube\ =\ 0.086m3$$

$Number\ of\ tubes\ required\ (Nt)\ =\ total\ volume/\ volume\ one\ tube$

$$\boldsymbol{Nt = \frac{Total\ Volume\ of\ Reactor}{Volume\ of\ one\ tube} = 43}$$

5) *Diameter of Shell*:

As,

$$\boldsymbol{Nt = \frac{\left[(Ds-K1)^2 * \frac{\pi}{4} + K2\right] - Pt * (Ds-K1) * (nK3+K4)}{1.223 * (Pt)^2}} \qquad (5.25)$$

Where,

$Nt\ =\ number\ of\ tubes$

$Ds\ =\ Shell\ Dia$

$K1, K2, K3, K4$ *are Constants based on tube size and shape.*

$Pt\ =\ pitch\ (1.25 * Tube\ Diameter)$

$n\ =\ number\ of\ tube\ passes$

After mathematical manipulation of the above equation we get,

---

[34] Bulk Density of Catalyst = 1300 (kg/m^3)

$$(1.223 * Pt_2) * Nt - (0.785) * K12 - (K1 * K3 * Pt * n) - (K1 * K4 * Pt) - K2 = (0.785 * D_{s2}) + (1.57 * K1 * Ds) - (Pt * Ds * K3 * n) - (Pt * K4 * Ds) \quad (5.26)$$

$$0.785 * Ds2 + 2.5061 * Ds - 2830.679 = 0$$

$$\boldsymbol{Ds = 58.46\ inch \qquad 1.5m}$$

6) $\boldsymbol{Height\ of\ the\ shell}$:

$$Tube\ Length^{35} = 4.876\ m$$

$Safety\ Holdup\ for\ TOP = 20\%$

$Safety\ Holdup\ for\ BOTTOM = 20\%$

$$\boldsymbol{Total\ height\ of\ shell = 6.82\ m}$$

$$\boldsymbol{Area\ of\ reactor = 1.73\ m^2}$$

7) **Pressure drops:**

$$\frac{\Delta P}{L} = [\frac{150*\mu*(1-\varepsilon)^2*uo}{\varepsilon^3*Dp^2*\varphi^2} + \frac{1.75*(1-\varepsilon)*\rho f*(uo)^2}{\varepsilon^3*Dp*\varphi}] \quad (5.27)$$

$Where,$

$\boldsymbol{\varepsilon} = Porosity$

$$\boldsymbol{\varphi = 0.58}$$

$\boldsymbol{\mu m} = Gaseous\ mixture\ Viscosity\ (Pa.s)$

$$\mu m = \frac{\sum_1^n \text{yi} * \mu i * (\sqrt{MW})}{\sum_1^n (yi * \sqrt{MW})}$$

$Dp = Diameter\ of\ particle\ (m)$

$\boldsymbol{\rho f} = Fluid\ Density\ (kg/m3)$

$\boldsymbol{uo} = Superficial\ Velocity^{36}\ (m.s)$

$$\Delta P = \left[\frac{150 * 2.5E-5 * (1-0.58)^2 * 2.311}{0.58^3 * 0.007^2 * 0.58^2} + \frac{1.75 * (1-0.58) * 1.861 * (2.3483)^2}{0.58^3 * 0.007 * 0.58}\right] * 4.87$$

$$\boldsymbol{\Delta P} = 48821.58\ Pa$$

$$\boldsymbol{\Delta P = 0.488\ bar}$$

---

[35] Tube Length = 16ft

[36] Superficial Velocity = (Volumetric Flowrate/Area)

Table 5.14: *Specification sheet of WGS Reactor*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	$R - 301$
Operation	Continuous
Type	Multi − tubular fixed bed reactor
Function	
Hydrogen synthesis through water − gas shift reaction	
Chemical reaction:	
$CO(g) + H_2O(v) \rightarrow CO_2(g) + H_2(g)$	
Catalyst	Fe − Al − Cu Size = 7 mm Weight of Catalyst = 2004 kg
Diameter of reactor	1.5 m
Volume of reactor	$4\ m^3$
Space time	1 sec
Number of tubes	43
Height of reactor	7 m
Area of reactor	$2\ m^2$
Pressure drop	0.5 bar

5.3. Design of steam tar reformer (TR-301):

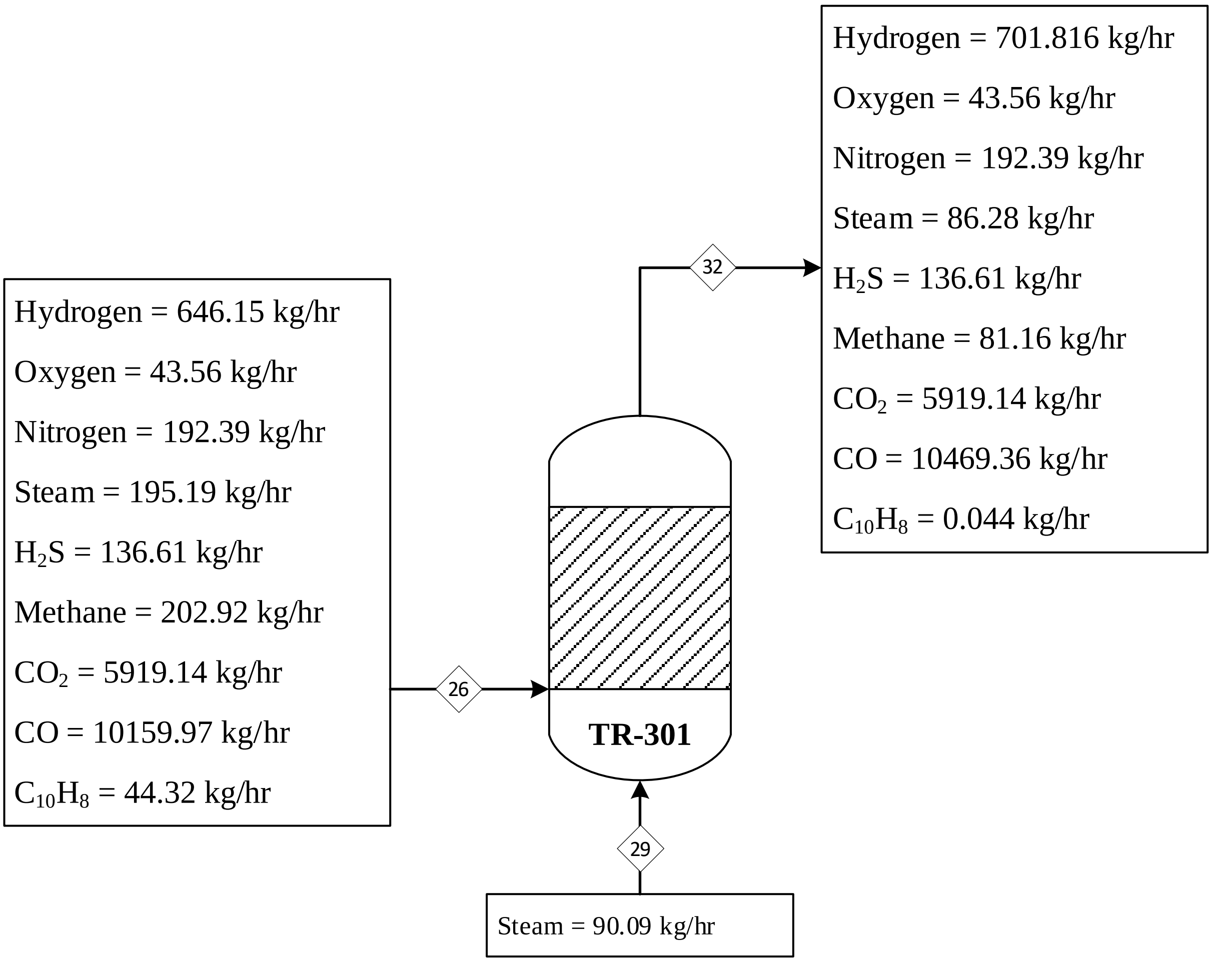


Figure 5.9: *Balance on tar reformer unit*

5.3.1. Design steps:

- Weight of Catalyst
- Volume of Catalyst
- Volume of Reactor
- Number of Tubes
- Diameter of Reactor
- Height of Reactor
- Pressure Drop

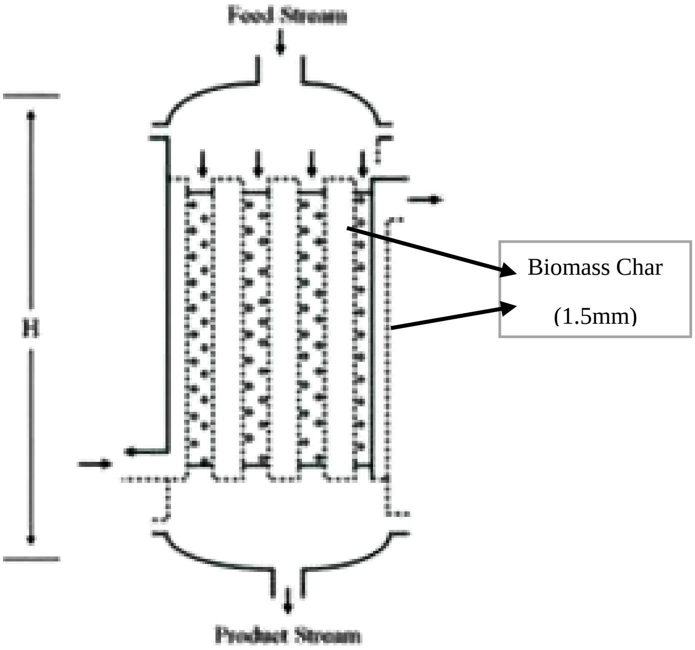


Figure 5.10: *Fixed bed reactor*

- **Operating conditions:**

$Temperature\ =\ 900\ °C$

$Pressure\ =\ 30\ bar$

$\boldsymbol{Reaction\ (01)}$:

$$C_{10}H_8\ (g)\ +\ 10H_2O\ (v)\ \rightarrow\ 10CO_2\ (g)\ +\ 14H_2\ (g) \qquad (5.28)$$

$\boldsymbol{Reaction\ (02)}$:

$$CH4\ (g)\ +\ H2O\ (v)\ \rightarrow\ CO\ (g)\ +\ 3H2\ (g) \qquad (5.29)$$

- $\boldsymbol{Calculation\ procedure}$:

$\boldsymbol{Performance\ equation\ of\ PBR}$:

$$\frac{W}{Fao} = \int_0^{Xa} \frac{dXa}{(-ra)} \qquad (5.30)$$

- $\boldsymbol{For\ reaction\ (01)}$

Kinetic equation: [55]

$$(-r_{tar}) = k_{app} * C_{tar} \qquad (5.31)$$

For variable density system,

$Initial\ Volume = 11\ (Total\ stoichiometric\ moles\ of\ reactant)$

$Final\ Volume = 24\ (Total\ stoichiometric\ moles\ of\ product)$

$$\varepsilon = \frac{\boldsymbol{(Final\ Volume - Initial\ Volume)}}{\boldsymbol{Initial\ Volume}} \Rightarrow \frac{\mathbf{(24-11)}}{\mathbf{11}}$$

$$\boldsymbol{\varepsilon\ =\ 1.18}$$

Table 5.15: *Terminologies used in tar reformer reactor.*

Component	**Mass flow (kg/hr.)**	**Molar Flowrate (kmol/hr.)**	**Mole Fraction**	**Density (kg/m^3)**	**Volumetric Flowrate[37] (m^3/hr)**
H_2	646.15	320.51	0.37	0.620	1042.05
O_2	43.56	1.36	0.0015	9.842	4.42
N_2	192.39	6.87	0.008	8.612	22.34
Water	285.26	15.83	0.0184	5.541	51.48
H_2S	136.61	4.006	0.0046	10.488	13.02
CH_4	202.92	12.65	0.0147	4.933	41.13
CO_2	5919.14	134.49	0.156	13.536	437.27
CO	10159.97	362.72	0.421	8.615	1179.29
Naphthalene	44.32	0.34	0.00040	39.422	1.12
Sum	17630.37	858.80	1		

- $\boldsymbol{Density\ of\ gaseous\ mixture}$:

$$\rho m = \frac{\sum_1^n \rho_i * \dot{V_i}}{\sum_1^n \dot{V}_i} \tag{5.32}$$

- $\boldsymbol{Volumetric\ flowrate\ of\ mixture}$:

$$\dot{V} = \frac{\dot{m}}{\rho i}$$

$$\mathbf{\dot{V} = 2792.14\ (m^3/hr)}$$

Or by $\boldsymbol{P\dot{V} = \dot{n} * RT}$

$$\mathbf{\dot{V} = 2792.14\ (m^3/hr)}$$

$As, F_{ao} = C_{ao} * \dot{V}, where\ F_{ao}\ is\ initial\ molar\ feed\ rate\ (kmol/hr).$
$So, Concentration\ from\ the\ above\ relation\ comes\ out\ to\ be,$

---

[37] R(m3.bar/K.mol) = 8.31E-05

Table 5.16: *Concentration of components used.*

Component	Concentration (kmol/m^3)
Napthalene ($C_{10}H_{8}$,o)	0.000123868
Steam (C_{H2O},o)	0.005657357
Carbon Dioxide (Cco_2,o)[38]	0.002718717
Hydrogen ($C_{H2,o}$)	0.008156152

1) $\boldsymbol{Weight\ of\ catalyst}$:

$$\frac{W}{Fao} = \int_0^{Xa} \frac{dXa}{(-ra)}$$

To draw the Levenspiel plot, convert the kinetic equation into form that consists of rate as function of conversion.

So,

$$-r_{C_{10}H_8} \; = \; ko * exp(-Ea/RT) * C_{tar} \tag{5.33}$$

$Where,$

$$C_{tar} \; = \; C_{ao} * (1 - Xa)/(1 + \mathcal{E}aXa) \tag{5.34}$$

$ko \; = \; 1.10E + 4\ sec - 1$

$Ea \; = \; 61\ (KJ/mol)$

$R \; = \; 0.008314\ (KJ/mol.K)$

$So,$

$$(-r_{C_{10}H_8})^{39} \; = \; ko * exp(-Ea/RT) * C_{ao} * (1 - Xa)/(1 + 1.18Xa) \tag{5.35}$$

$By\ applying\ Simpson's\ Quadrature\ formula\ i.e.,$

$$\int_{\boldsymbol{Xo}}^{\boldsymbol{X4}} \boldsymbol{f(X)dX} = \frac{\boldsymbol{h}}{\boldsymbol{3}} * (\boldsymbol{f(xo) + 4f(x1) + 2f(x2) + 4f(x3) + f(x4)}) \tag{5.36}$$

Table 5.17: *Solving rate equation of reaction 1*

Xa	(-ra)	1/(-ra)
0	0.00261	381.749
0.2475	0.00152	655.696
0.495	0.00083	1198.165
0.7425	0.00035	2783.438
0.99	1.20715E-05	82843.736

---

[38] Product outlet molar flow is found by moles produced from a particular reaction.

[39] Rate is written in (kmol/m^3.sec)

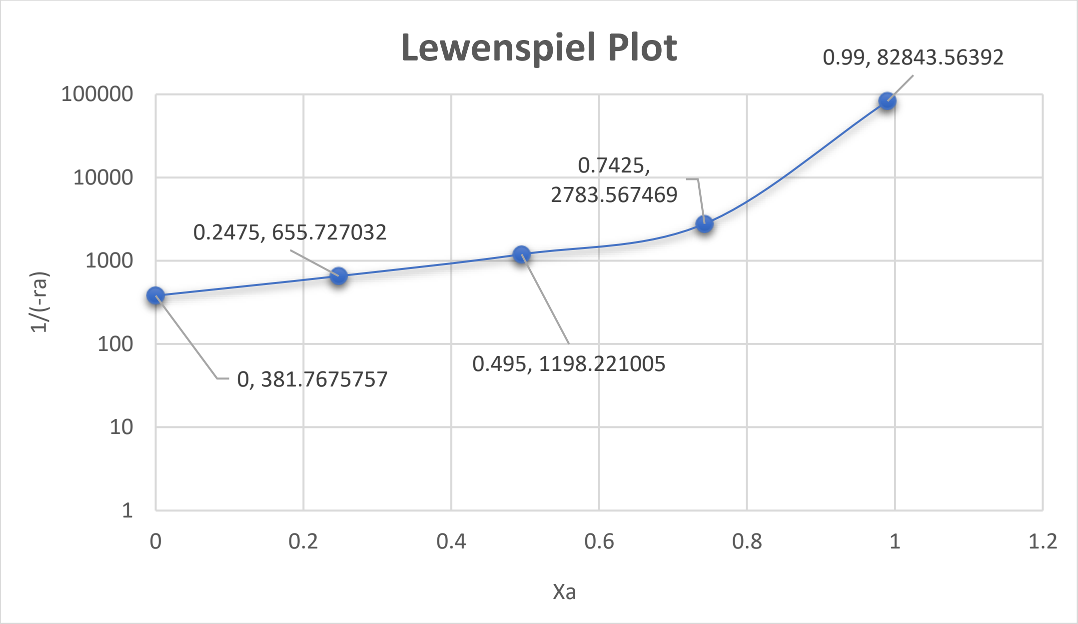


Figure 5.11: *Levenspiel plot of reaction 1*

$$Catalyst\ Used: \boldsymbol{Biomass\ Char} Weight\ of\ Catalyst\ (kg) = (Area\ under\ the\ curve) * \left(\frac{\boldsymbol{Fao}}{\boldsymbol{3600}}\right) * (Cao) * (MWC10H8) = (8198) * \left(\frac{\mathbf{0.348}}{\mathbf{3600}}\right) * (0.000123) * (128.17) \tag{5.37}$$

$$\boldsymbol{Weight\ of\ \ catalyst\ (kg)\ =\ 0.012}$$

- $\boldsymbol{For\ reaction\ (02)}$

$$CH4\ (g)\ +\ H2O\ (v)\ \ \rightarrow\ \ CO\ (g)\ +\ 3H2\ (g)$$

$\boldsymbol{Kinetic\ equation}$:

$$r = \frac{krxn*\sqrt{PH2O}*\sqrt{PCH4}}{(1+\sqrt{KCH4*PCH4})+(1+KH2O*PH2O)^2} \tag{5.38}$$

$Where,$

- $krxn\ (mol * Kpa/m^2 * s)\ =\ 1.55E-05$
- $KCH_4\ (Kpa^{-a})\ =\ 5.33E-02$
- $KH_2O\ (Kpa^{-B})\ =\ 1.40E-02$
- $R\ (m^3.Kpa/mol.K)\ =\ 0.008314$
- $PCH_4\ =\ 44.1953 * ((1-Xa)/(1+\varepsilon a * Xa))$
- $PH_2O\ =\ (Ch2o,0 - Cch4,o * Xa)/(1+\varepsilon b * Xb)$

$$\frac{\boldsymbol{Cao} * \mathbf{Xa}}{\boldsymbol{a}} = \frac{\boldsymbol{Cbo} * \mathbf{Xb}}{\boldsymbol{b}}$$

$Xb\ =\ 0.80 * Xa$

For variable density system,

$Initial\ Volume = 2\ (Total\ stoichiometric\ moles\ of\ reactant)$

$Final\ Volume = 4\ (Total\ stoichiometric\ moles\ of\ product)$

$$\varepsilon a = \frac{\boldsymbol{(Final\ Volume - Initial\ Volume)}}{\boldsymbol{Initial\ Volume}} \Rightarrow \frac{\mathbf{(4-2)}}{\mathbf{2}}$$

$$\boldsymbol{\varepsilon a\ =\ 1}$$

As,

$$\frac{\boldsymbol{a} * \boldsymbol{\varepsilon}\mathbf{a}}{\boldsymbol{Cao}} = \frac{\boldsymbol{b} * \boldsymbol{\varepsilon}\mathbf{b}}{\boldsymbol{Cbo}}$$

So, from the above equation, εb =1.24

Table 5.18: *Concentration of component used tar reformer.*

Component	Concentration (mol/m^3)
Methane ($C_{H_4,o}$)	4.530985956
Steam ($C_{H_2O,o}$)	5.671307402
Carbon Monoxide ($C_{co,o}$)[40]	1.226234835
Hydrogen ($C_{H_2,o}$)	1.716728769

- **Weight of catalyst:**

$$\frac{W}{Fao} = \int_0^{Xa} \frac{dXa}{(-ra)}$$

Incorporating the variable density term into the concentration term and writing rate as a function of Conversion we get,

$$\boldsymbol{r}^{41} = \frac{\mathbf{1.55}\boldsymbol{E}\mathbf{-5}*\sqrt{\left(\mathbf{9.7535}*\left(\frac{\boldsymbol{CH20,o-Cch4,o*Xa}}{\mathbf{1+}\boldsymbol{\varepsilon b*Xb}}\right)\right)*\left(\mathbf{44.19}*\left(\frac{\mathbf{1-}\boldsymbol{Xa}}{\mathbf{1+}\boldsymbol{\varepsilon a*Xa}}\right)\right)}}{\left(\mathbf{1+}\sqrt{(\mathbf{5.33}\boldsymbol{E}\mathbf{-2})*\left(\mathbf{44.1953}*\left(\frac{\mathbf{1-}\boldsymbol{Xa}}{\mathbf{1+}\boldsymbol{\varepsilon a*Xa}}\right)\right)}\right)+\left(\mathbf{1+1.402}\boldsymbol{E}\mathbf{-2}*\left(\frac{\boldsymbol{CH2O,o-CcH4,o*Xa}}{\mathbf{1+}\boldsymbol{\varepsilon b*Xb}}\right)\right)^{\mathbf{2}}} \qquad (5.39)$$

Table 5.19: *Solving rate equation of reaction 2.*

Xa	(-ra)	1/(-ra)
0	0.000206998	4830.954712
0.15	0.000167222	5980.078363
0.3	0.000133424	7494.904079
0.45	0.00010392	9622.749733
0.6	7.74686E-05	12908.4518

---

[40] Product outlet molar flow is found by moles produced from a particular reaction

[41] Units of rate are (mol/m^2.sec)

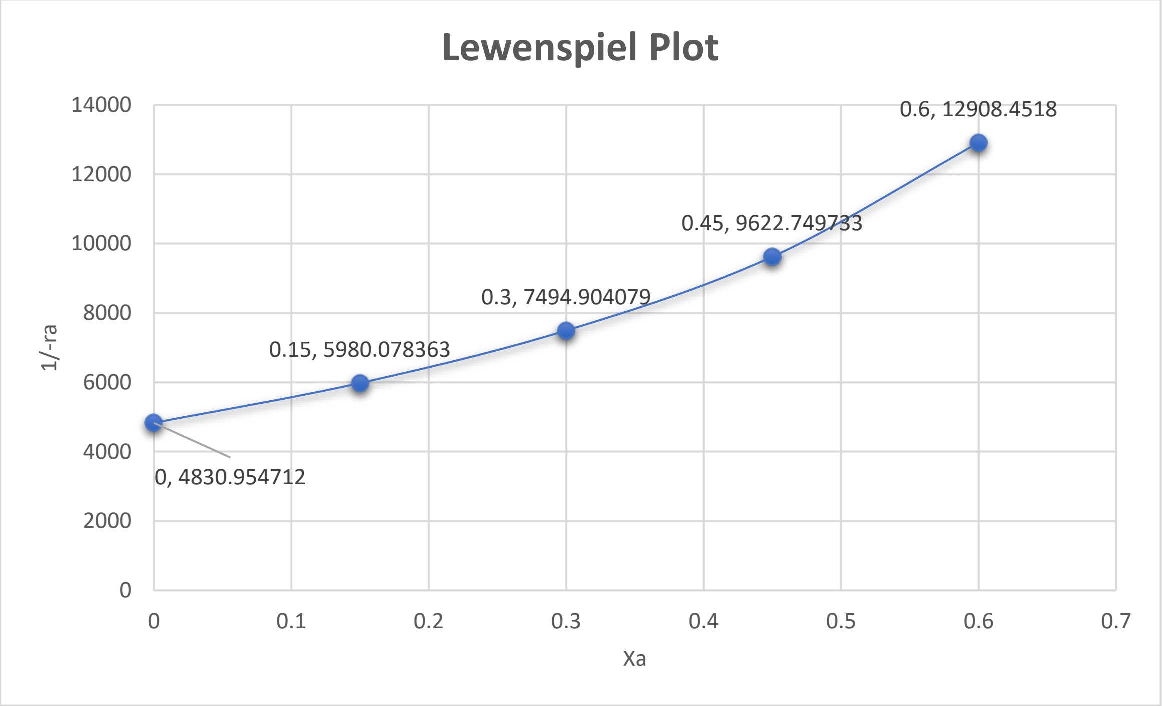


Figure 5.12: *Levenspiel plot of reaction 2*

$Weight\ of\ Catalyst\ (g)$

$$= (Area\ under\ the\ curve) * \left(\frac{F_{ao}}{3600}\right) * (C_{ao}) * (metal\ surface\ area) * 1000$$

$$= (4757.96) * (\frac{12.752}{3600}) * (3.4) * (1000)$$

$$\boldsymbol{Weight\ of\ catalyst\ (kg)\ =\ 57}$$

2) $\boldsymbol{Volume\ of\ catalyst}$:

$$Volume\ of\ Catalyst = \frac{Weight\ of\ Catalyst}{Bulk\ Density\ of\ Catalyst^{42}}$$

$$\boldsymbol{Volume\ of\ Catalyst\ =\ 0.10\ m^3}$$

3) $\boldsymbol{Volume\ of\ reactor}$:

$$Volume\ of\ reactor\ =\ Volume\ of\ Catalyst\ +\ Void\ Volume$$

$Also,$

$$\text{Volume of reactor} = \frac{\boldsymbol{Volume\ of\ Catalyst}}{\boldsymbol{1-\varepsilon}}$$

$\boldsymbol{\varepsilon}$ = 0.91

$$\boldsymbol{Volume\ of\ reactor\ =\ 1.21\ \mathrm{m}^3}$$

$As, space\ time\ is\ given\ by,$

$$\tau\ =\ (\frac{V}{\dot{V}})$$

$$\boldsymbol{\tau\ =\ 1.5\ sec}$$

4) $\boldsymbol{Number\ of\ tubes}$:

---

[42] Bulk Density of Catalyst = 520 (kg/m^3)

Let,
The nominal length of tubes be 16*ft*.
Dia of tube Dt be 10 *cm* (*should be between* (8 − 15) *cm due to accepted heuristics for plug flow in tubular reactor*)
Diameter of particles dp be 2.5 *mm*.
So,

$$\boldsymbol{\frac{Dt}{dp} = \frac{10*10}{1.5} = 40 \gg 15}\ (To\ avoid\ deviation\ from\ plug\ flow)$$

$$Volume\ of\ one\ tube\ = \boldsymbol{\pi * r^2 * L}$$

$$Volume\ of\ one\ tube\ = 0.038m3$$

Number of tubes required (*Nt*) = *total volume*/ *volume one tube*

$$\boldsymbol{Nt = \frac{Total\ Volume\ of\ Reactor}{Volume\ of\ one\ tube} = 32}$$

5) ***Diameter of shell***:

As,

$$\boldsymbol{Nt = \frac{\left[(Ds-K1)^2*\frac{\pi}{4}+K2\right]-Pt*(Ds-K1)*(nK3+K4)}{1.223*(Pt)^2}} \tag{5.40}$$

Where,
Nt = *number of tubes*
Ds = *Shell Dia*
*K*1, *K*2, *K*3, *K*4 *are Constants based on tube size and shape.*
Pt = *pitch* (1.25 ∗ *Tube Diameter*)
n = *number of tube passes*
After mathematical manipulation of the above equation we get,

$$(1.223 * Pt2) * Nt - (0.785) * K12 - (K1 * K3 * Pt * n) - (K1 * K4 * Pt) - K2 = (0.785 * Ds2) + (1.57 * K1 * Ds) - (Pt * Ds * K3 * n) - (Pt * K4 * Ds)$$

$$0.785 * Ds2 + 2.4521 * Ds - 946.15 = 0$$

$$\boldsymbol{Ds = 33.3\ inch \rightarrow 0.84m}$$

6) ***Height of the shell***:

$$Tube\ Length^{43} = 4.876\ m$$

Safety Holdup for TOP = 20%
Safety Holdup for BOTTOM = 20%

$$\boldsymbol{Total\ height\ of\ Shell = 6.82m}$$

$$\boldsymbol{Area\ of\ Reactor = 0.56\ m2}$$

7) ***Pressure drop***:

$$\frac{\Delta P}{L} = [\frac{150*\mu(1-\varepsilon)^2*uo}{\varepsilon^3*Dp^2*\varphi^2} + \frac{1.75*(1-\varepsilon)*\rho f*(uo)^2}{\varepsilon^3*Dp*\varphi}] \tag{5.41}$$

Where,
$\boldsymbol{\varepsilon}$ = *Porosity*

---

[43] Tube Length = 16ft

$\boldsymbol{\mu m} = \ Gaseous\ mixture\ Viscosity\ (Pa.s)$

$$\mu m = \frac{\sum_1^n \mathrm{yi} * \mu i * \left(\sqrt{MW}\right)}{\sum_1^n \left(yi * \sqrt{MW}\right)}$$

$Dp\ =\ Diameter\ of\ particle\ (m)$

$\boldsymbol{\rho f}\ =\ Fluid\ Density\ (kg/m3)$

$\boldsymbol{uo} = \ Superficial\ Velocity^{44}\ (m.s)$

$$\Delta P = \left[\frac{150 * 2.7E - 5 * (1 - 0.91)^2 * 1.379}{0.91^3 * 0.0025^2 * 0.87^2} + \frac{1.75 * (1 - 0.91) * 6.314 * (1.379)^2}{0.91^3 * 0.0025 * 0.87}\right] * 4.87$$

$$\Delta P\ =\ 5692.3\ Pa$$

$$\boldsymbol{\Delta P\ =\ 0.05\ bar}$$

---

[44] Superficial Velocity = (Volumetric Flowrate/Area)

Table 5.20: *Specification sheet of tar reformer*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	TR – 301
Operation	Continuous
Type	Multi – tubular fixed bed reactor
Function	
Carbon monoxide synthesis through hydrocarbons reforming	
Chemical reaction:	
$C_{10}H_8\ (g) + 10H_2O\ (v) \rightarrow 10CO_2\ (g) + 14H_2\ (g)$ $CH_4\ (g) + H_2O\ (v) \rightarrow CO\ (g) + 3H_2\ (g)$	
Catalyst	Biomass Char Size = 2.5 mm Weight of Catalyst = 58 kg
Diameter of reactor	0.8 m
Volume of reactor	1.2 m^3
Space time	2 sec
Number of tubes	32
Height of reactor	7 m
Area of reactor	0.6 m^2
Pressure drop	0.05 bar

5.4. Design of fluidized bed gasifier (G-201):

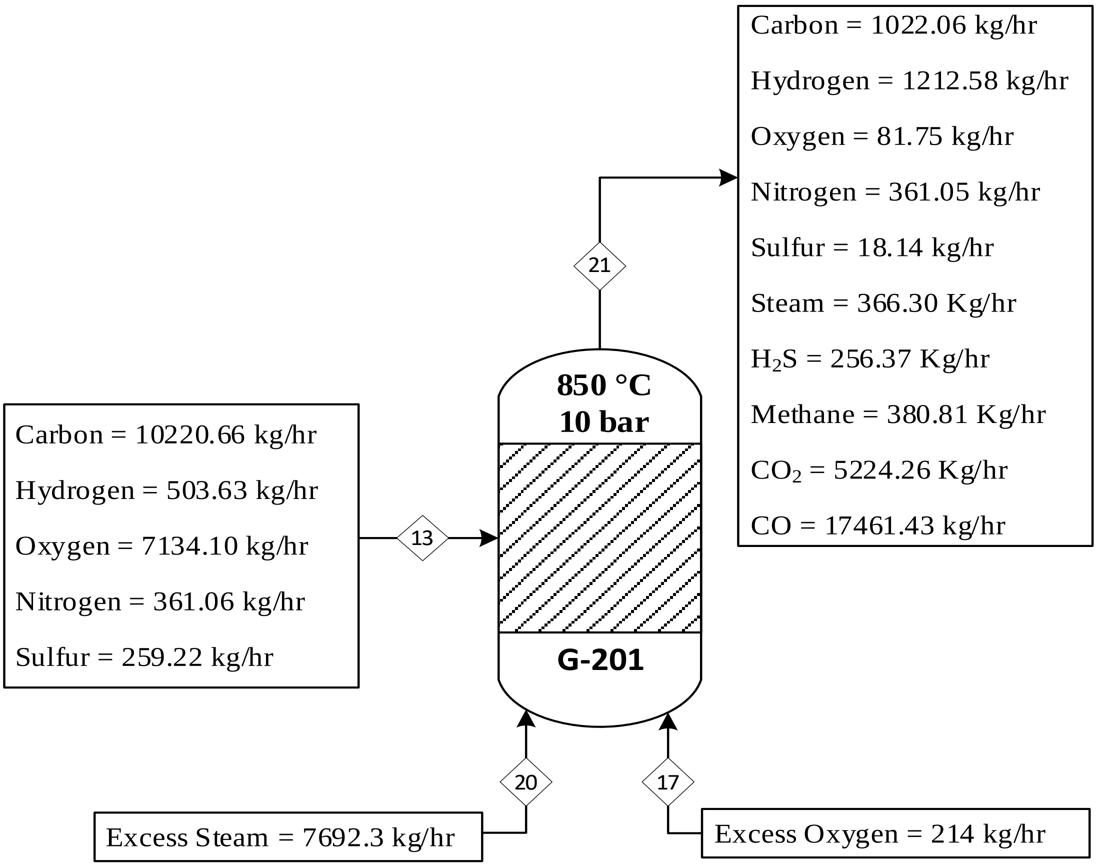


Figure 5.13: *Balance on gasifier unit*

5.4.1. Design steps: [56]

- Minimum Fluidization Velocity (U_{mf})
- Operating Velocity (U_f)
- Selection of Fluidization Regime
- Slugging Velocity (U_s)
- Static Bed Height (L_{mf})
- Terminal Velocity (U_t)
- Reactor Height and Residence Time

- ***Operating conditions***:

$Temperature\ =\ 850\,°C$

$Pressure\ =\ 10\ bar$

- ***Reactions***:

$$C(s)\ +\ H_2O(v)\ \rightarrow\ CO(g)\ +\ H_2(g) \tag{5.42}$$

$$C(s)\ +\ O_2(g)\ \rightarrow\ CO_2\ (g) \tag{5.43}$$

$$C(s)\ +\ 2H_2(v)\ \rightarrow\ CH_4(g) \tag{5.44}$$

$$S(s) +\ H_2(v)\ \rightarrow\ H_2S\ (g) \tag{5.45}$$

$$C(s)\ +\ \frac{1}{2}O_2(g)\ \rightarrow\ CO_2\ (g) \tag{5.46}$$

- ***Calculation procedure***:

1) ***Catalyst specifications***:

Catalyst Bulk density = 1400 ($kg/m3$)
Fluid Average density = 0.1435 ($kg/m3$)
Diameter of solid particles = 0.5 *mm*
Sphericity of particles = 0.78
Porosity of particle = 0.57

2) ***Minimum fluidization velocity***:

$$Umf = \frac{dp^2*(\rho s-\rho g)*g}{150\mu} * \frac{emf^3*\varphi s^2}{1-emf} \tag{5.47}$$

Where,
Umf = Minimum fluidization velocity of the particles within the bed.
dp is the diameter of the particle,
ρs and ρg are the densities of the particle and fluid respectively,
g is the acceleration due to gravity,
εmf is the voidage fraction of particle
ɸs is the sphericity of the particle.
By plugging in the appropriate values, the minimum fluidization velocity comes out to be

$$\boldsymbol{Umf = 0.272\ m/s}$$

3) ***Operating velocity***:

$$\frac{H}{Hmf} = 1 + \frac{10.978*(Uf-Umf)^{0.738}*\rho s^{0.376}*dp^{1.006}}{Umf^{0.937}*\rho g^{0.126}} \tag{5.48}$$

Where,

$$\boldsymbol{1.2 < \frac{H}{Hmf} < 1.4}\ (Taking\ H/Hmf\ to\ be\ 1.3\ and\ solving\ for\ Uf)$$

$$\boldsymbol{Uf = 1.10\ (m/s)}$$

4) ***Characterizing the fluidizing regime***:

In order to map out the fluidization regime, two dimensionless quantities are calculated,

$$u^* = Uf\left(\frac{\rho g^2}{\mu*(\rho s-\rho g)g}\right)^{\frac{1}{3}} \tag{5.49}$$

$$dp^* = dp\left(\frac{\rho g*(\rho s-\rho g)g}{\mu^2}\right)^{\frac{1}{3}} \tag{5.50}$$

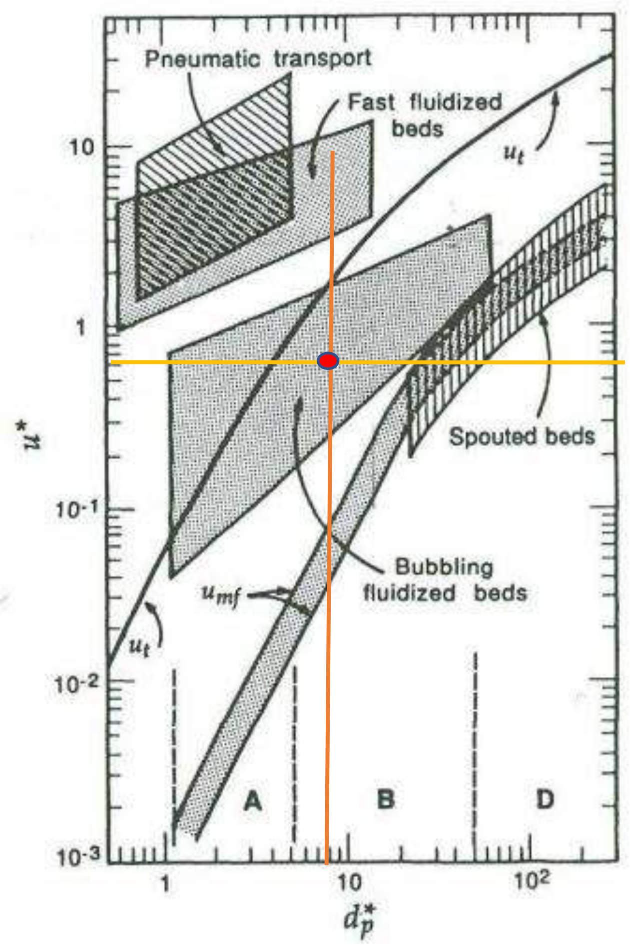


Figure 5.14: *Selection of gasifier bed* [57]

So,

$$\boldsymbol{u}^* = \mathbf{0.45}$$
$$\boldsymbol{dp}^* = \mathbf{8}$$

Based on the particle size velocity, according to above, provided by Kunii and Levenspiel, these conditions dictate the flow regime of the bed to be a bubbling fluidized bed.

5) $\boldsymbol{Slugging\ velocity}$:

$First\ calculate\ the\ cross-sectional\ area\ of\ reactor\ by,$

$$\dot{m}f = 6E-7*A*P \qquad (5.51)$$

$Where,$

$\boldsymbol{\dot{m}f}\ =\ mass\ flowrate\ of\ fuel$[45]

$\boldsymbol{A}\ =\ Cross-sectional\ area\ of\ reactor$

$\boldsymbol{P}\ =\ Absolute\ Pressure$

$From\ the\ above\ relation,$

$$\boldsymbol{A\ =\ 4.41\ m^2}$$

$Now\ as\ Area\ =\boldsymbol{\frac{\pi}{4}}*\boldsymbol{D^2}.So, diameter\ of\ reactor\ equals\ to,$

$$\boldsymbol{D\ =\ 2.37\ m}$$

$For\ Slugging\ velocity,$

$$Us = Umf + 0.07*(g*D)^{0.5} \qquad (5.52)$$

---

[45] Includes only those reactants that are taking part in reaction

$$\boldsymbol{Us\ =\ 0.60\ m/s}$$

$The\ maximum\ bed\ height\ below\ which\ the\ bed\ will\ be\ freely\ bubbling\ is\ calculated\ by,$

$$Hfb^{46} = \frac{D-2.51*D^{0.2}}{0.13*D^{0.47}} \tag{5.53}$$

$$\boldsymbol{Hfb\ =\ 135.1\ cm}$$

$The\ Height\ at\ which\ complete\ SLUGGING\ sets\ in$

$$Zs = 60D^{0.175} \tag{5.54}$$

$$\boldsymbol{Zs\ =\ 156.22\ cm}$$

This means slugging would occur if the fluidized substance reached the height more than 135.1cm. So, the maximum fluidization height would be 135.1 cm because after that slugging would start and causes adverse pressure gradients inside the reactor.

6) ***Static bed height***:

$$\frac{Lf}{Lmf} = 1 + [10.978 * (Uf - Umf)^{0.738} * dp^{1.006} * Umf^{-0.937} * \rho f^{-0.126}] \tag{5.55}$$

$Where,$

$Lmf\ =\ Static\ Bed\ Heght.$

$Lf\ or\ Hfb\ =\ Height\ below\ which\ freely\ bubbling\ occurs.$

$So, solving\ for\ static\ bed\ height\ in\ the\ above\ equation,$

$$\boldsymbol{Lmf\ =\ 97.21\ cm}$$

7) ***Terminal velocity***:

$Terminal\ Velocity\ for\ irregular\ shaped\ particles\ are\ given\ by,$

$$ut^* = \left[\frac{18}{(dp^*)^2} + \frac{2.335-1.744\varphi s}{(dp^*)^{\left(\frac{1}{2}\right)}}\right]^{-1} \tag{5.56}$$

$So,$

$$\boldsymbol{ut^*\ =\ 1.60}$$

Now

$$Ut = \frac{ut^*}{\left(\frac{\rho g^2}{\mu*(\rho s-\rho g)*g}\right)^{\frac{1}{3}}} \tag{5.57}$$

$$\boldsymbol{Ut = 3.89\ m/s}$$

8) ***Reactor height***:

As L/D for bubbling fluidized bed is in between 2 to 10. Taking Length as twice of diameter we have,

$L\ =\ 4.74\ m, and$

$Volume\ of\ gasifier^{47}\ =\ 21\ m^3$

$Space\ time\ =\ 5.6\ seconds$

9) ***Distributor plate design***:

- ***Bed pressure drop***:

$$\Delta Pb =\ \rho s * Lmf * (1 - \varepsilon mf) * g \tag{5.58}$$

$Where,$

$\Delta \boldsymbol{P_b} =\ Pressure\ drop\ in\ the\ bed.$

---

[46] Where Diameter of reactor is in cm

[47] V = π *r²*L

$$\boldsymbol{\Delta P_b = 5735.26\ Pa}$$

- $\boldsymbol{Distributor\ Plate\ Pressure\ Drop}$:

$$\boldsymbol{\Delta P_d = 0.30 * \Delta Pb}$$

$So,$

$$\boldsymbol{\Delta P_d = 1720.58\ Pa}$$

10) $\boldsymbol{Superficial\ gas\ velocity\ through\ Orifice}$:

$$Uor = Cd * \sqrt{\frac{2\Delta Pd}{\rho g}} \qquad (5.59)$$

$Where,$

$Cd = 0.6\ (coefficient\ of\ discharge)$

$$\boldsymbol{Uor = 92.88\ m/s}$$

- $\boldsymbol{Diameter\ of\ orifice}$:

$$\boldsymbol{dor = 3 * dp}$$

$$\boldsymbol{dor = 1.5mm}$$

- $\boldsymbol{Number\ of\ orifices\ per\ square\ meter}$:

$$Nor = \left(\frac{Uf}{Uor}\right) * \left(\frac{4}{\pi * dor^2}\right) \qquad (5.60)$$

$Number\ of\ orifices\ per\ square\ meter\ (Nor) = 6698$

$Let\ pitch\ be\ triangular, and\ so\ for\ triangular\ pitch\ configuration,$

$$P = \frac{1}{\sqrt{Nor * \sin(60^0)}} \qquad (5.61)$$

$From\ the\ above\ formula,$

$$\boldsymbol{P = 0.0140\ m}$$

- $\boldsymbol{To\ avoid\ bubble\ coalescence}$:

$$P = \left(\frac{1}{g^{\frac{1}{5}}}\right) * \left[\frac{6 * (Uf - Umf)}{\pi Nor}\right]^{\frac{2}{5}} \qquad (5.62)$$

$So,$

$$\boldsymbol{P = 0.022 \geq 0.02}$$

- $\boldsymbol{For\ avoiding\ stagnant\ zones}$:

$$P = dor + \left(\frac{Uf - Umf}{30.1 * Nor}\right)^{\frac{1}{0.716 * dp^{0.205}}} \qquad (5.63)$$

$$\boldsymbol{P = 0.0015 \leq 1.7}$$

Table 5.21: *Specification sheet of gasifier*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	$G-201$
Operation	Continuous
Type	Bubbling fluidized bed gasifier
Function	
Syngas formulation via solid waste gasification	
Chemical reactions:	
$C(s) + H_2O(v) \rightarrow CO(g) + H_2(g)$ $C(s) + O_2(g) \rightarrow CO_2\,(g)$ $C(s) + 2H_2(v) \rightarrow CH_4(g)$ $S(s) + H_2(v) \rightarrow H_2S\,(g)$ $C(s) + \frac{1}{2}O_2(g) \rightarrow CO_2\,(g)$	
Catalyst	Calcined Dolomite Size $= 0.5\ mm$
Diameter of reactor	$2.5\ m$
Space time	6 seconds
Volume of reactor	$21\ m^3$
Height of reactor	$5\ m$
Number of orifices	6698
Pressure drop	$0.05\ bar$

5.5. Design of scrubber (S-301):

The removal of one or many constituents from a gaseous mixture using a suitable solvent is the second important mass transfer operation in Chemical Engineering. Soluble vapors are absorbed in the gas absorption process. A solvent derived from a combination of inert gas and a solvent. The goal of this type of gas scrubbing is to remove contaminants from the synthesis gas.

Any of the following operations are possible:

- **i.** For the separation of components with monetary worth.
- **ii.** As a step in the manufacturing of a chemical.
- **iii.** To get rid of an unwanted component (pollution).

- **Types of absorption:**

i. Physical absorption

Mass transfer occurs solely by diffusion in physical absorption, and physical absorption is regulated by physical equilibria.

ii. Chemical absorption

A chemical reaction occurs when a specific component comes into touch with the absorbing liquid then, by lowering the concentration of the component in the liquid phase, the rate of diffusion is increased.

Table 5.22: *Comparison between types of absorbers.*

Packed column	Plate column
It provides continuous contact between vapours and liquid phases.	It brings the two phases into contact on stage wise basis.
Pressure drop in packed column is less than the plate column and less liquid hold up. So, it makes the unit as compact as possible for safety.	In plate column, Pressure drop, and liquid hold up is high because of additional friction generated as the vapor passes through the liquid on each tray.
For column diameter of less than approximately 8 ft, it is more usual to employ packed towers because it is cost effective.	High fabrication cost of small trays
Packed columns are more suitable for handling foaming and Corrosive systems.	Plate columns are often used to foul fouling liquids or solids
Liquid hold in packed column is lower because in packed tower the liquid flow as a thin film over the packing.	Because of the liquid on each plate there may be an Urge quantity of liquid in Plate Column.

- **Type of packing:**

A packed column is chosen as the absorber based on the preceding considerations. Because the solubility of a liquid is infinite, it will absorb as many gases as it comes into contact with, hence a densely packed tower will give more contact. It is simple to use.

Principal Requirement of a Tower packing are:

- **a)** It must be chemically inert to the tower's fluids.
- **b)** It must be sturdy without being overly heavy.
- **c)** It must have enough channels for both streams to flow freely without causing undue liquid hold-up or pressure decrease.
- **d)** It must allow for good liquid-to-gas interaction.
- **e)** It must be cost-effective.

As a result, most packaging is constructed of inexpensive, inert, and relatively light materials like clay, porcelain, or graphite. Some limes are thin-walled metal rings made of steel or aluminum.

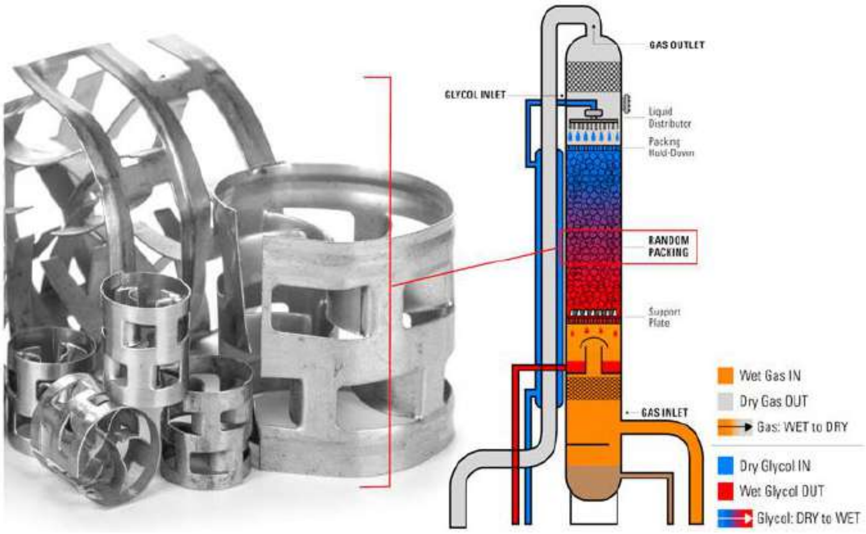


Figure 5.15: *Absorption column*

- **Classes of packing:**
  They can be divided into two broad classes:
  1) **Packing with a regular geometry:** such as stacked rings, grids and proprietary structured packings.
  2) **Random packings:** rings, saddles and proprietary shapes, which are dumped into the column and take up a random arrangement.

Figure 5.16: *Structured and random packing*

- **Common packing’s:**
  a. Berl Saddle.
  b. Intalox Saddle.
  c. Rasching rings.
  d. Lessing rings.
  e. Cross-partition rings.
  f. Single spiral ring.
  g. Double - Spiral ring.
  h. Triple - Spiral ring.

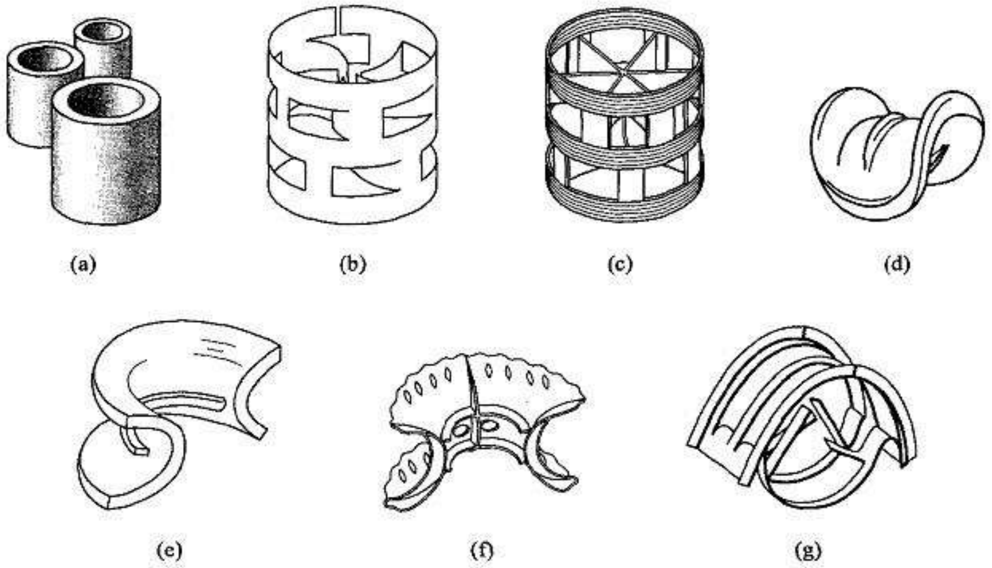
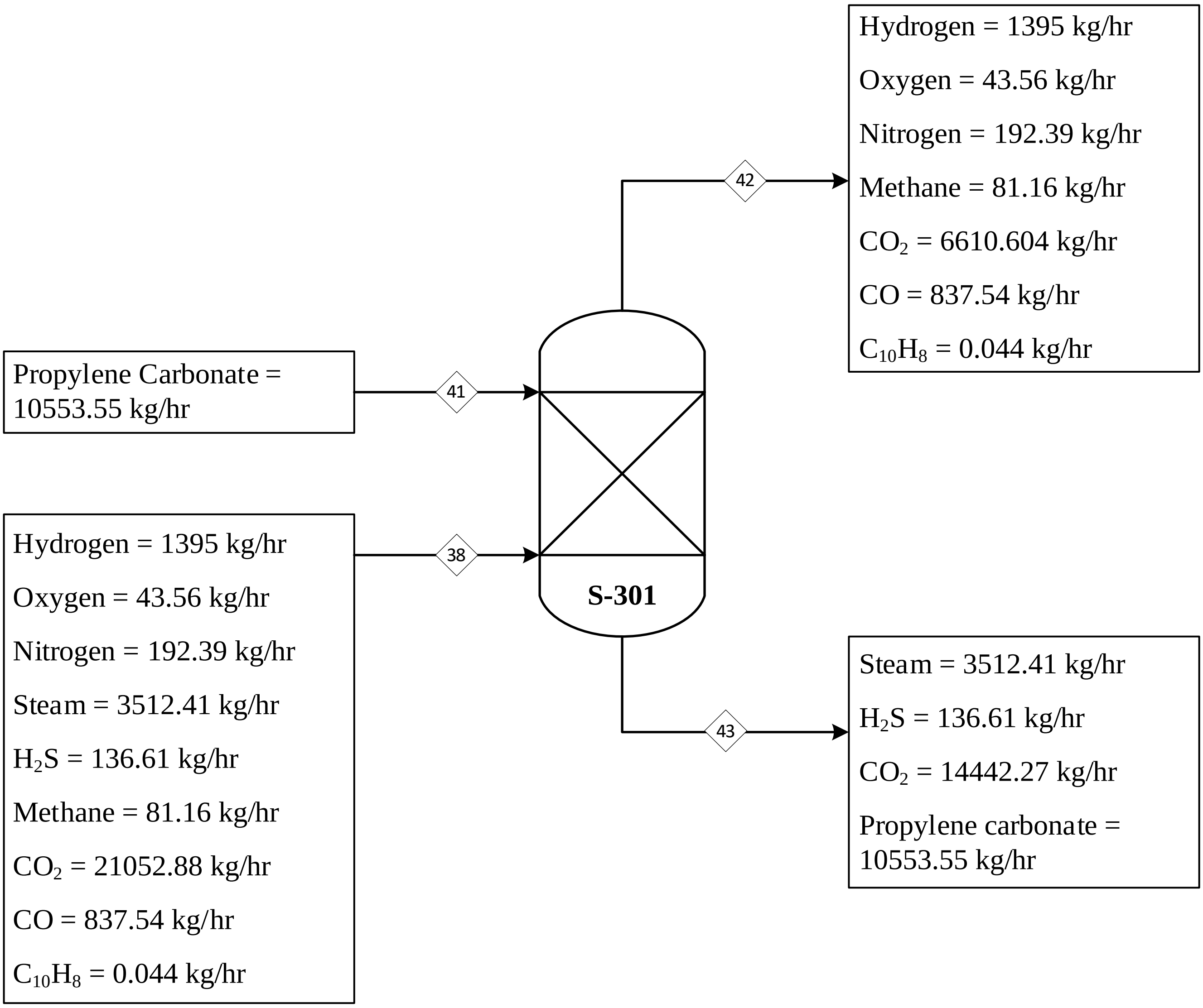


Figure 5.17: *(a) Raschig rings (b) Metal pall rings (c) Plastic pall rings (d) Berl saddle ceramic (e) Intalox saddle ceramic (f) Plastic super intalox saddle (g) Metal intalox saddle*



Hydrogen = 1395 kg/hr
Oxygen = 43.56 kg/hr
Nitrogen = 192.39 kg/hr
Methane = 81.16 kg/hr
CO_2 = 6610.604 kg/hr
CO = 837.54 kg/hr
$C_{10}H_8$ = 0.044 kg/hr

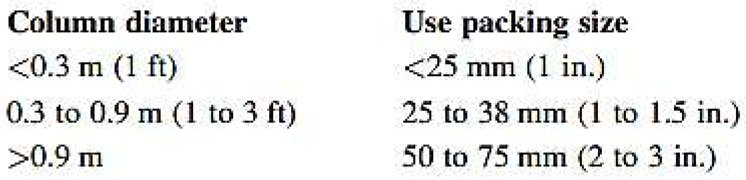
Propylene Carbonate = 10553.55 kg/hr

Hydrogen = 1395 kg/hr
Oxygen = 43.56 kg/hr
Nitrogen = 192.39 kg/hr
Steam = 3512.41 kg/hr
H_2S = 136.61 kg/hr
Methane = 81.16 kg/hr
CO_2 = 21052.88 kg/hr
CO = 837.54 kg/hr
$C_{10}H_8$ = 0.044 kg/hr

Steam = 3512.41 kg/hr
H_2S = 136.61 kg/hr
CO_2 = 14442.27 kg/hr
Propylene carbonate = 10553.55 kg/hr

Figure 5.18: *Balance on scrubber (S-301)*

- Recommended size ranges are:



Column diameter	Use packing size
<0.3 m (1 ft)	<25 mm (1 in.)
0.3 to 0.9 m (1 to 3 ft)	25 to 38 mm (1 to 1.5 in.)
>0.9 m	50 to 75 mm (2 to 3 in.)

5.5.1. Design steps:

1) Select the type and size of packing.
2) Calculation of Flow Factor $F_{LV.}$
3) Calculation of Diameter of column.
4) Calculation of height of transfer units Z.
5) Calculation of Liquid film Mass transfer Coefficient $K_{L.}$
6) Calculation of gas film Mass transfer Coefficient $K_{G.}$
7) Calculation of gas film transfer unit height $H_{OG.}$
8) Calculate number of overall gas-phase transfer units $N_{OG.}$
9) Calculation of flooding velocity $\boldsymbol{F_{vl}}$.
10) Calculation of height of tower Z.
11) Calculation of wetting rate.
12) Calculation for Operating velocity $F_{LV.}$
13) Calculation of Pressure drop.

5.5.2. Design calculation:

1) $\boldsymbol{Selection\ of\ packing}$:

We Choose INTALOX® saddles ceramic due to:

- Provide a large Interfacial surface area between liquid and gas.
- Random packing is usually cost, corrosion resistant, have a low-pressure drop.
- We are dealing with Corrosive System so that’s why we use Ceramic based material to improve the efficiency.

It is the most crucial aspect of the scheme. The packaging allows enough space for close contact between the phases. The total size of the tower is largely determined by the efficiency of packaging in terms of both HTU and flow volume. As a result, the packing option affects the installation's economics.

The packaging is separated into two types: those that are poured into the tower at random and those that must be stacked by hand. Dumped packing has a major dimension of 1/4 to 3 inches and is used in the smaller columns, whereas stacked packing has a major dimension of 2 to around 8 inches and is used only in the larger towers.

2) $\boldsymbol{Flow\ factor\ (F_{LV})}$:

The relation for flow factor is.

$$F_{LV} = \frac{\dot{L}}{\dot{G}}\sqrt{\frac{\rho_g}{\rho_L}} = 0.045 \qquad (5.64)$$

Where,

$Flowrate\ of\ entering\ gas = G = 7.57\ {}^{kg}/_{s}$

$Flowrate\ of\ entering\ slovent = L = 2.93\ {}^{kg}/_{s}$

$Design\ for\ 42\ mm\ of\ \frac{H_2O}{m}\ of\ packing\ height\ (Ray\ Sinnott\ Vol\ 6)$

$k_4 = 1.74\ \ at\ pressure\ drop\ (From\ fig\ 11.44\ )$

- $\boldsymbol{Diameter\ of\ column}$:

$$\boldsymbol{G^{*}} = \left[\frac{\boldsymbol{K_4\rho_g(\rho_L-\rho_g)}}{\boldsymbol{131F_P(^{\mu_L}/_{\rho_L})^{0.1}}}\right]^{\boldsymbol{0.5}} = 8.49\, \boldsymbol{kg}/\boldsymbol{m^2.sec} \qquad (5.65)$$

G^{*} = *gas mas flow-rate per unit column cross-sectional area (kg/*$m^2.sec$*)*

$Viscosity\ of\ liquid(solvent) = \mu_L = 0.0019\ Pa.s\ \&\ (\frac{kg}{m.sec})$

$Viscosity\ of\ gas\ mixture = \mu_g = 0.000032\ Pa.s\ \&\ (\frac{kg}{m.sec})$

$Density\ \ of\ liquid(solvent) = \rho_L = 1182.23\ \frac{kg}{m^3}$

$Density\ of\ gas\ mixture = \rho_g = 15.92\ kg/m^3$

$\boldsymbol{Packing\ parameter\ for\ 2-inch\ ceramic\ intalox\ saddles = Fp = 130\ m^{-1}}$

$$\boldsymbol{A = \frac{G}{G^{*}} = \frac{7.57}{8.49} = 0.89\ m^2}$$

$$\boldsymbol{Diameter\ of\ column = D = \sqrt{\frac{4\times A}{\pi}} = 1.07\ m}$$

3) $\boldsymbol{Calculation\ of\ height\ of\ transfer\ units\ (HTU)}$:

Using Onda Method:

- **Effective interficial area ($\boldsymbol{a_w}$):**

$$\frac{a_w}{a} = 1 - exp\left[-1.45\left(\frac{\sigma_c}{\sigma_L}\right)^{0.75}\left(\frac{L_W}{a\mu_L}\right)^{0.1}\left(\frac{L_W{}^2a}{\rho_{2L}g}\right)^{-0.05}\left(\frac{L_W}{\rho_L\sigma_L a}\right)^{0.2}\right] \qquad (5.66)$$

a_w = Effective interficial area of packing per unit volume = $m^2/_{m^3}$

a = Actual area of packing per unit volume = 108 $m^2/_{m^3}$ (Table 11.2)

σ_c = Critical surface tension for $material$ = 0.061 N/m (Standard for Ceramic Packing)

L_W =Liquid mass velocity = 3.29 $\frac{kg}{m^2S}$

$Density\ \ of\ liquid(solvent) = \rho_L = 1182.23\ \frac{kg}{m^3}$

μ_L = Viscosity of Liquid = 0.0019 Pa. s & $(\frac{kg}{m.sec})$

σ_L = Liquid Surface Tension = 0.0433 N/m

$$\boldsymbol{a_w = 64.24\ {}^{m^2}/_{m^3}}$$

4) $\boldsymbol{Calculation\ of\ liquid\ film\ mass\ transfer\ coefficient\ (K_L)}$:

$$K_{L:}\left[\frac{\rho_L}{\mu_L g}\right]^{1/3} = 0.0051\left[\frac{L_W}{a_w\mu_L}\right]^{2/3}\left[\frac{\mu_L}{\rho_L D_c}\right]^{-1/2}[adp]^{0.4} \qquad (5.67)$$

$K_L =\ liquid\ film\ coefficient\ \ (\frac{m}{s})$

$d_p =\ packing\ size\ =\ 51\ mm\ =\ \ 51\ \times 10^{-3}\ m\ (source: Table\ 11.2)$

$D_L = Diffusivity\ of\ liquid\ (solvent) = 6.35\times10^{-9}\ m^2/s\ (Source: Literature)$

$\rho_L =\ 1182.23\ kg\ /\ m^3$

$a = Actual\ area\ of\ packing\ per\ unit\ volum = 108\ \ m^2\ /\ m^{\ 3}\ \ (source: Table\#11.2)$

$L_w =\ 3.29\ kg/(m^2\ S)$

$\mu_L = 0.0019\ Pa.s\ \&\ (\frac{kg}{m.sec})$

$g = 9.8\ m/s$

$$K_L = 1.43 \times 10^{-4}\ m/s$$

5) $\boldsymbol{Calculation\ of\ gas\ film\ mass\ transfer\ coefficient\ (K_G):}$

$$K_G \frac{RT_g}{D_g a} = K_5 \left[\frac{V_W}{a\mu_g}\right]^{0.7} \left[\frac{\mu_g}{\rho_g D_g}\right]^{1/3} [adp]^{-2} \qquad (5.68)$$

$K_5 = 5.23\ for\ packing\ above\ 15\ mm$
$V_W = 8.48\ kg/(m^2\ S)$
$a = Actual\ area\ of\ packing\ per\ unit\ volum = 108\ m^2\ /\ m^3\ \ (Table\ \#11.2)$
$D_g = Diffusivity\ of\ gases = 2.01 \times 10^{-6}\ m^2/s$
$d_p = packing\ size = 51\ mm = 51 \times 10^{-3}\ m$
$\rho_g = 15.92\ kg\ /\ m^3$
$T_g = 437.15\ °K$
$\mu_g = 0.000032\ \ Pa.s\ \&\ (\frac{kg}{m.sec})$
$R = 0.08314\ (bar\ m^3)\ /\ (kmol.K)$

$$\mathbf{K_G = 2.43 \times 10^{-4}\ ^{kmol}/_{m^2.s.bar}}$$

6) $\boldsymbol{Gas\ film\ transfer\ unit\ height\ (HG):}$

$$H_G = \frac{G_m}{K_g a_w P} \qquad (5.69)$$

$G_m = Gas\ mass\ velocity = 0.440\ \ kmol/m^2\ .s$
$P_g = Pressure\ of\ gases = 30\ bar$
$K_G = Gas\ film\ coefficient = 2.43 \times 10^{-4}\ kmol/m^2.s.bar$
$a_w = Effective\ interfacial\ area\ of\ packing\ per\ unit\ volume = 64.24\ \ m^2/m^3$

$$\boldsymbol{H_G = 0.94\ m}$$

7) $\boldsymbol{Calculation\ of\ liquid\ transfer\ unit\ height\ (HL):}$

$$H_L = \frac{L_m}{K_L a_w C_t} \qquad (5.70)$$

$L_m = Liquid\ mass\ velocity = 0.032\ \ kg/m^2\ .s$
$C_t = Total\ Concentration = \rho_L\ /\ Molecular\ weight\ of\ solvent = 11.580\ kmol/m^3$
$K_L = Liquid\ \ film\ coefficient = 1.43 \times 10^{-4}\ m/s$
$a_W = Effective\ interfacial\ area\ of\ packing\ per\ unit\ volume = 64.24\ m^2/m^3$

$$\boldsymbol{H_L = 0.302\ m}$$

8) $\boldsymbol{Calculation\ of\ height\ of\ an\ overall\ gas-phase\ transfer\ unit\ (HOG):}$

$$H_{OG} = H_G - \frac{mG_m}{L_m} \times H_L \qquad (5.71)$$

$H_G = 0.94\, m$

$H_L = 0.302\, m$

$\frac{mG_m}{L_m} = 0.75$ (Range 0.7 – 0.8)

$$\boldsymbol{H_{OG} = 1.166\, m}$$

9) *Equation for equilibrium curve*:

$\boldsymbol{y_1}$ = mole fraction of Solute in gas Entering Stream (loading specific H_2S & CO_2) = $\mathbf{0.4795}$

$\boldsymbol{y_2}$ = mole fraction of Solute in gas leaving Stream (loading specific H_2S & CO_2) = $\mathbf{0.1234}$

$\boldsymbol{y_1}/\boldsymbol{y_2}$ = 0.4795 / 0.1234 = 3.89

10) *Calculation of number of overall gas – phase transfer units* (*NOG*)

$$N_{OG} = \frac{1}{1-(m\frac{G_m}{L_m})} ln\, [\left(1 - \frac{mG_m}{L_m}\right)\frac{y_1}{y_2} + \frac{mG_m}{L_m}] \qquad (5.72)$$

$$\boldsymbol{N_{OG} = 2.17}$$

Or (**From Fig 11.40**)

$$N_{OG} = 2.2$$

11) *Calculation of height of tower*:

$$z = N_{OG} \times H_{OG} \qquad (5.73)$$

$\boldsymbol{H_{OG}}$ = 1.166 $\boldsymbol{m}$

$\boldsymbol{N_{OG}}$ = 2.17

$$\boldsymbol{Z = 2.53\ \ m}$$

Allowance for liquid distribution & redistribution = 1.0 m + 1.0 m = 2 m

$$\boldsymbol{z = 4.53\, m}\ \textbf{(15 ft)}$$

12) *Calculation of wetting rate*:

$$wetting\ rate = \frac{volumetric\ flowrate}{a} = \mathbf{2.57 \times 10^{-5}}\, \boldsymbol{{m^2}/{s}} \qquad \textbf{(5.74)}$$

$volumetric\ liquid\ flowrate = 0.0028\ {m^3}/{s}$

a = Actual area of packing per unit volume = $108\, {m^2}/{m^3}$

- ***Operating velocity*:**

$$F_{vl} = \frac{L}{G}\sqrt{\frac{\rho_g}{\rho_l}} = \mathbf{0.045}$$

k_4 *at design pressure* = 1.74 (*From fig* 11.54)

$$G^* = [\frac{K_4\rho_g(\rho_L - \rho_g)}{131F_P({\mu_L}/{\rho_L})^{0.1}}]^{0.5} = \mathbf{4.25}\ \boldsymbol{{kg}/{m^2.s}}$$

- ***Flooding velocity*:**

$$F_{vl} = \frac{L}{G}\sqrt{\frac{\rho g}{\rho l}} = \mathbf{0.045}$$

k_4 *at flooding line* = 4.12 (*From fig* 11.54)

$$G^* = [\frac{K_4\rho_g(\rho_L - \rho_g)}{131F_P({\mu_L}/{\rho_L})^{0.1}}]^{0.5} = \mathbf{13.06}\ \boldsymbol{{kg}/{m^2.s}}$$

- $\% \boldsymbol{Flooding}$:

$$\% \boldsymbol{Flooding} = \sqrt{\frac{\boldsymbol{K_4\ at\ design\ pressure\ drop}}{\boldsymbol{K_4\ at\ flooding}}} = \mathbf{65}\ \% \qquad (5.75)$$

13) $\boldsymbol{Pressure\ drop\ \Delta P}$:

- $\boldsymbol{Pressure\ drop\ at\ flooding}$:

$$\Delta P = 0.115\ F_p^{\ 0.7} \qquad (5.76)$$

$Packing\ parameter\ for\ 2 - inch\ ceramic\ intalox\ saddles = Fp = 130\ m^{-1}$

$$\Delta P = 3.47\ (in\ H_2O/m\ packing)$$

$$\boldsymbol{\Delta P = 88.16\ (mm\ H_2O/m\ packing)}$$

- $\boldsymbol{Pressure\ drop\ across\ column}$:

$Using\ Figure\ 18.6: (source:\ McCabe\ Smitt)$

$$\frac{G_L}{G_g}\sqrt{\frac{\rho_g}{\rho_l - \rho_g}} = \mathbf{0.045}$$

and

$$\frac{G_g F_p \mu_L^{0.1}}{g_c(\rho_L - \rho_g)\rho_g} = \mathbf{0.0084}$$

From Figure Using Appendix A:

$$\boldsymbol{\Delta P = 0.067\ \left(inch \frac{H_2O}{ft} packing\right)}$$

$0.067\ (inch\ H_2O)$	$25.39\ (mm\ H_2O)$	$3.28\ ft$
ft	$1\ (inch\ H_2O)$	$1\ m$

$$\boldsymbol{\Delta P = 5.58\ (mm\ H_2O/m\ packing)}$$

$$\Delta P_{Column} = 5.58 \times Z$$

$\boldsymbol{\Delta P_{Column}}$= 5.58 × $\mathbf{4.53}$

$$\Delta P = 26.46\ mm\ H_2O$$

$$\boldsymbol{\Delta P = 0.0026\ bar}$$

Table 5.23: *Specification sheet of scrubber*

Specification Sheet	
Identification	
Item	Scrubber
Item #	$S-301$
Operation	Continuous
Type	Packed Column
Packing	INTALOX® saddles ceramic
Function	
To absorb the H_2S, CO_2 gas from process Stream	
Operating Pressure	$30\ bar$
Operating Temperature	$437.15\ °K$
Diameter	$1.07\ m$
Effective Interfacial Area of packing	$64.24\ (m^2/m^3)$
height of an overall gas − phase transfer unit (H_{OG})	$1.166\ m$
number of overall gas − phase transfer units (N_{OG})	2.17
Height of Transfer Unit	$2.54\ m$
Total Height	$4.54\ m$
Pressure drop (ΔP)	$0.0377\ psi$

5.6. Design of stripper (ST-301):

It is a counter-current multi-stage at the bottom stage separation column, with liquid feed at top stage and vapor feed at the bottom stage.

- **Stripping phenomenon:**

Stripping is a mass transfer operation that involves the transfer of a solute (as H_2S & CO_2 in our case) from the liquid phase to the gas phase.

"Stripping is a unit operation where one or more components of a liquid stream are removed by being placed in contact with a gas stream that is insoluble in the liquid stream."

Basically, Stripping is a physical separation process where one or more components are removed from a liquid stream by a vapor stream. In industrial applications the liquid and vapor streams can have co-current or counter current flows. Stripping is usually carried out in either a packed or tray column.

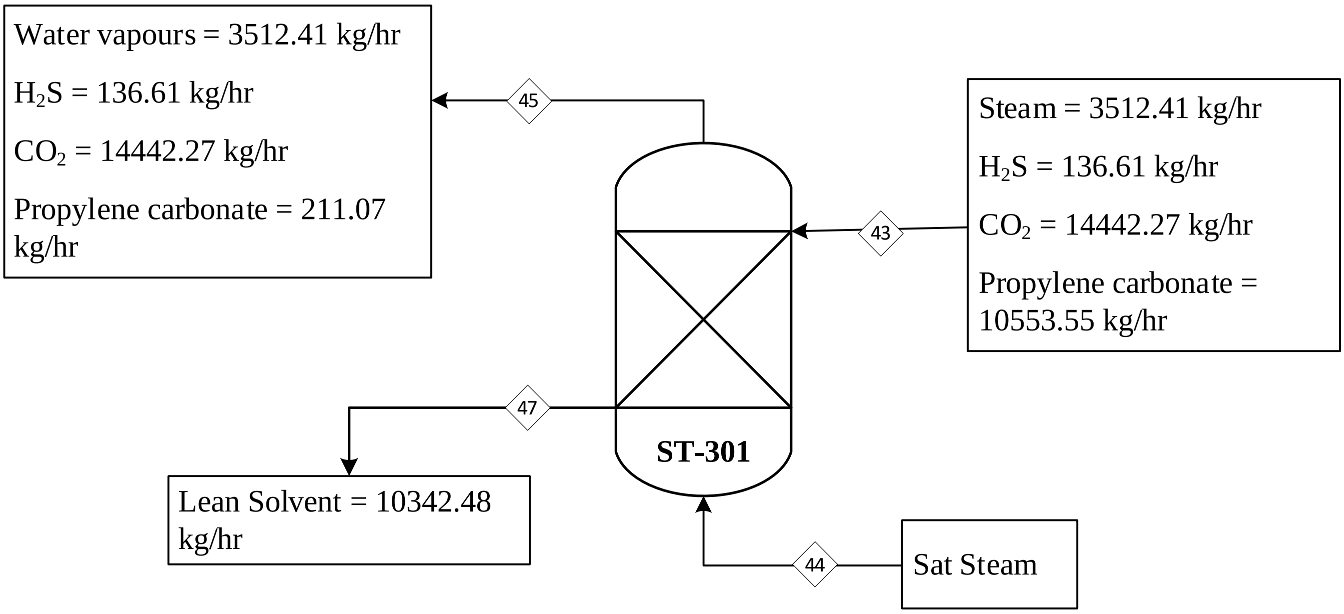


Figure 5.19: *Balance on stripper (ST-301)*

5.6.1. Design steps:

1) Select the type and size of packing.
2) Calculation of Diameter of column.
3) Calculation of Liquid film Mass transfer Coefficient $K_{L.}$
4) Calculation of gas film Mass transfer Coefficient $K_{G.}$
5) Calculation of gas film transfer unit height $H_{OG.}$
6) Calculate number of overall gas-phase transfer units $N_{OG.}$
7) Calculation of height of tower Z.
8) Calculation of wetting rate.
9) Calculation of Pressure drop.

5.6.2. Design calculation:

1) ***Selection of packing***:

We Choose INTALOX® saddles ceramic due to:

- Provide a large Interfacial surface area between liquid and gas.
- Random packing is usually cost, corrosion resistant, have a low-pressure drop.
- We are dealing with Corrosive System so that’s why we use Ceramic based material to improve efficiency.

2) $\boldsymbol{Flow\ factor\ (F_{LV})}$:

The relation for flow factor is.

$$F_{LV} = \frac{L}{G}\sqrt{\frac{\rho_g}{\rho_L}} = \mathbf{0.090}$$

Where,

$Flowrate\ of\ entering\ gas = G = 5.03\ {}^{kg}/_{s}$

$Flow\ rate\ of\ entering\ slovent = L = 2.93\ {}^{kg}/_{s}$

$Design\ for\ 42\ mm\ of\ \frac{H_2O}{m}\ of\ packing\ height\ (Ray\ Sinnott\ Vol\ 6)$

$k_4 = 1.47\ at\ pressure\ drop\ (From\ fig\ 11.44)$

3) $\boldsymbol{Diameter\ of\ column}$:

$$G^* = \left[\frac{K_4\rho_g(\rho_L - \rho_g)}{131F_P\left({}^{\mu_L}/_{\rho_L}\right)^{0.1}}\right]^{0.5} = \mathbf{10.35}\ {}^{\boldsymbol{kg}}/_{\boldsymbol{m^2.sec}}$$

G^* = *gas mass flow-rate per unit column cross-sectional area (kg/m*^{2}*. sec)*

$Viscosity\ of\ liquid(solvent) = \mu_L = 0.0019\ Pa.s\ \&\ (\frac{kg}{m.sec})$

$Viscosity\ of\ gas\ mixture = \mu_g = 0.00125\ Pa.s\ \&\ (\frac{kg}{m.sec})$

$Density\ of\ liquid(solvent) = \rho_L = 1182.23\ \frac{kg}{m^3}$

$Density\ of\ gas\ mixture = \rho_g = 28.33\ kg/m^3$

$Packing\ parameter\ for\ 2-inch\ ceramic\ intalox\ saddles = Fp = 130\ m^{-1}$

$$A = \frac{G}{G^*} = \frac{7.57}{8.49} = \mathbf{0.49\ m^2}$$

$$Diameter\ of\ column = D = \sqrt{\frac{4 \times A}{\pi}} = \mathbf{0.79\ m}$$

4) $\boldsymbol{Calculation\ of\ height\ of\ transfer\ units\ (HTU)}$:

Using Onda Method:

- **Effective interficial area ($\boldsymbol{a_w}$):**

$$\frac{a_w}{a} = 1 - exp\left[-1.45\left(\frac{\sigma_c}{\sigma_L}\right)^{0.75}\left(\frac{L_W}{a\mu_L}\right)^{0.1}\left(\frac{Lw^2a}{\rho_{2L}g}\right)^{-0.05}\left(\frac{L_W}{\rho_L\sigma_L a}\right)^{0.2}\right]$$

a_w = Effective interficial area of packing per unit volume = ${}^{m^2}/_{m^3}$

a = Actual area of packing per unit volum = 108 ${}^{m^2}/_{m^3}$ (Table 11.2)

σ_c = Critical surface tension for *material* = 0.061 N/m (Standard for Ceramic Packing)

L_W =Liquid mass velocity = 6.03 $\frac{kg}{m^2S}$

$Density\ of\ liquid(solvent) = \rho_L = 1182.23\ \frac{kg}{m^3}$

μ_L = Viscosity of Liquid = 0.0019 Pa. s & ($\frac{kg}{m.sec}$)

σ_L = Liquid Surface Tension = 0.0433 N/m

$$\boldsymbol{a_w = 73.87 \, {}^{m^2}/_{m^3}}$$

5) $\boldsymbol{Calculation\ of\ liquid\ film\ mass\ transfer\ coefficient\ (K_L)}$:

$$K_{L:}\left[\frac{\rho_L}{\mu_L g}\right]^{1/3} = 0.0051\left[\frac{L_W}{a_w \mu_L}\right]^{2/3}\left[\frac{\mu_L}{\rho_L D_c}\right]^{-1/2}[adp]^{0.4}$$

$K_L = liquid\ film\ coefficient\ (\frac{m}{s})$

$d_p = packing\ size\ =\ 51\ mm\ =\ 51\ \times 10^{-3}\ m\ (source: Table\ 11.2)$

$D_L = Diffusivity\ of\ liquid\ (solvent) = 6.35 \times 10^{-9}\ m^2/s\ (Source: Literature)$

$\rho_L =\ 1182.23\ kg\ /\ m^3$

$a = Actual\ area\ of\ packing\ per\ unit\ volume\ = 108\ \ m^2\ /\ m\ ^3\ (source: Table\ 11.2)$

$L_w =\ 6.03\ kg/(m^2\ S)$

$\mu_L = 0.0019\ Pa.s\ \&\ (\frac{kg}{m.sec})$

$g = 9.8\ m/s$

$$\boldsymbol{K_L = 1.96 \times 10^{-4}\ m/s}$$

6) $\boldsymbol{Calculation\ of\ gas\ film\ mass\ transfer\ coefficient\ (K_G)}$:

$$K_G \frac{RT_g}{D_g a} = K_5\left[\frac{V_W}{a\mu_g}\right]^{0.7}\left[\frac{\mu_g}{\rho_g D_g}\right]^{1/3}[adp]^{-2}$$

$K_5 = 5.23\ for\ packing\ above\ 15\ mm$

$V_W =\ 10.34\ \ kg/(m^2\ S)$

$a =\ Actual\ area\ of\ packing\ per\ unit\ volume = 108\ m^2\ /\ m^3\ \ (Table\ 11.2)$

$D_g = Diffusivity\ of\ gases = 4.42 \times 10^{-5}\ m^2/s$

$d_p =\ packing\ size\ =\ 51\ mm\ =\ 51 \times 10^{-3}\ m$

$\rho_g =\ 28.3\ kg\ /\ m^3$

$T_g = 437.15\ °K$

$\mu_g = 0.001253\ Pa.s\ \&\ (\frac{kg}{m.sec})$

$R = 0.08314\ (bar\ m^3)\ /\ (kmol.K)$

$$\mathbf{K_G = 4.72 \times 10^{-4}\ {}^{\boldsymbol{kmol}}/_{\boldsymbol{m^2.s.bar}}}$$

7) $\boldsymbol{Gas\ film\ transfer\ unit\ height\ (H_G)}$:

$$H_G = \frac{G_m}{K_g a_w P}$$

$G_m\ =\ Gas\ mass\ velocity\ =\ 0.301\ \ kmol/m^2\ .s$

$P_g\ =\ Pressure\ of\ gases\ =\ 30\ bar$

$K_G =\ Gas\ film\ coefficient\ =\ 4.72 \times 10^{-4}\ kmol/m^2.s.bar$

$a_w\ =\ Effective\ interfacial\ area\ of\ packing\ per\ unit\ volume\ =\ 73.87\ \ m^2/m^3$

$$\boldsymbol{H_G\ =\ 0.288\ m}$$

8) $\boldsymbol{Calculation\ of\ liquid\ transfer\ unit\ height\ (HL)}$:

$$H_L = \frac{L_m}{K_L a_w C_t}$$

$L_m = Liquid\ mass\ velocity = 0.059\ kg/m^2\ .s$
$C_t = Total\ Concentration = \rho_L\ /\ Molecular\ weight\ of\ solvent = 11.580\ kmol/m^3$
$K_L = Liquid\ film\ coefficient = 1.96 \times 10^{-4}\ m/s$
$a_W = Effective\ interfacial\ area\ of\ packing\ per\ unit\ volume = 73.87\ m^2/m^3$

$$\boldsymbol{H_L = 0.353\ m}$$

9) $\boldsymbol{Calculation\ of\ height\ of\ an\ overall\ gas - phase\ transfer\ unit\ (HOG)}$:

$$H_{OG} = H_G - \frac{mG_m}{L_m} \times H_L$$

$H_G = 0.288\ m$
$H_L = 0.353\ m$
$\frac{mG_m}{L_m} = 0.75$ (Range0.7 – 0.8)

$$\boldsymbol{H_{OG} = 0.553\ m}$$

- $\boldsymbol{Equation\ for\ equilibrium\ curve}$:

$\boldsymbol{y_1}$ = mole fraction of Solute in Solvent Entering Stream (loading specific H_2S & CO_2) = $\boldsymbol{0.836}$
$\boldsymbol{y_2}$ = mole fraction of Solvent in Solvent leaving Stream (loading specific H_2S & CO_2) = $\boldsymbol{0.179}$

$$\boldsymbol{y_1/y_2} = 0.836 / 0.179 = 4.66$$

10) $\boldsymbol{Calculation\ of\ number\ of\ overall\ gas - phase\ transfer\ units\ (NOG)}$

$$N_{OG} = \frac{1}{1-(m\frac{G_m}{L_m})} \ln\left[\left(1 - \frac{mG_m}{L_m}\right)\frac{y_1}{y_2} + \frac{mG_m}{L_m}\right]$$

$$\boldsymbol{N_{OG} = 2.60}$$

Or (**From Fig 11.40**)

$$N_{OG} = 2.58$$

11) $\boldsymbol{Calculation\ of\ height\ of\ Tower}$:

$$z = N_{OG} \times H_{OG}$$

$\boldsymbol{H_{OG}} = 0.553\ \boldsymbol{m}$
$\boldsymbol{N_{OG}} = 2.58$

$$\boldsymbol{Z = 1.44\ m}$$

$Allowance\ for\ liquid\ distribution\ \&\ redistribution = 1.0\ \text{m} + 1.0\ \text{m} = 2\ \text{m}$

$$\boldsymbol{z = 3.44\ m\ (11.5\ ft)}$$

12) $\boldsymbol{Calculation\ of\ wetting\ rate}$:

$$wetting\ rate = \frac{volumetric\ flow\ rate}{a} = \boldsymbol{4.73 \times 10^{-5}\ m^2/s}$$

$volumetric\ liquid\ flowrate = 0.0051\ m^3/s$

a = Actual area of packing per unit volume = $108\ m^2/m^3$

- **Operating velocity:**

$$F_{vl} = \frac{L}{G}\sqrt{\frac{\rho_g}{\rho_l}} = \mathbf{0.091}$$

$k_4\ at\ design\ pressure\ = 1.47\ (From\ fig\ 11.54)$

$$G^* = [\frac{K_4\rho_g(\rho_L-\rho_g)}{131F_P({}^{\mu_L}/_{\rho_L})^{0.1}}]^{0.5} = \mathbf{10.35}\ {}^{\boldsymbol{kg}}/_{\boldsymbol{m^2.s}}$$

- $\boldsymbol{Flooding\ velocity}$:

$$F_{vl} = \frac{L}{G}\sqrt{\frac{\rho g}{\rho l}} = \mathbf{0.091}$$

$k_4\ at\ flooding\ line = 3.58\ (From\ fig\ 11.54)$

$$G^* = [\frac{K_4\rho_g(\rho_L-\rho_g)}{131F_P({}^{\mu_L}/_{\rho_L})^{0.1}}]^{0.5} = \mathbf{16.15}\ {}^{\boldsymbol{kg}}/_{\boldsymbol{m^2.s}}$$

- **Percentage flooding:**

$$\%\ Flooding\ = \sqrt{\frac{K_4\ at\ design\ pressure\ drop}{K_4 at\ flooding}} = \mathbf{64.08}\ \%$$

13) $\boldsymbol{Pressure\ drop\ \Delta P}$:

- $\boldsymbol{Pressure\ drop\ at\ Flooding}$:

$$\Delta P = \ 0.115\ F_p{}^{0.7}$$

$Packing\ parameter\ for\ 2-inch\ ceramic\ intalox\ saddles = Fp = 130\ m^{-1}$

$$\Delta P\ =\ 3.47\ (in\ H_2O/m\ packing)$$

$$\boldsymbol{\Delta P\ =\ 88.16\ (mm\ H_2O/m\ packing)}$$

- $\boldsymbol{Pressure\ drop\ across\ column}$:

$For\ Pressure\ drop\ we\ using\ Figure\ 18.6$: $(source$: $McCabe\ Smitt)$

Hence,

$$\frac{G_L}{G_g}\sqrt{\frac{\rho_g}{\rho_l-\rho_g}} = \mathbf{0.091}$$

and

$$\frac{G_gF_p\mu_L^{0.1}}{g_c(\rho_L-\rho_g)\rho_g} = \mathbf{0.0071}$$

From Figure Using Appendix B:

$$\Delta P = 0.062\ \left(inch\frac{H_2O}{ft}packing\right)$$

$0.062\ (inch\ H_2O)$	$25.39\ (mm\ H_2O)$	$3.28\ ft$
ft	$1\ (inch\ H_2O)$	$1\ m$

$$\boldsymbol{\Delta P = 5.16\ (mm\frac{H_2O}{m}\ packing)}$$

$$\Delta P_{Column} = 5.16 \times Z$$

ΔP_{Column}= 5.16×3.44

$$\Delta P = 17.76\ mm\ H_2O$$

$$\boldsymbol{\Delta P = 0.0017\ bar}$$

Table 5.24: *Specification sheet of stripper*

Specification Sheet	
Identification	
Item	*Scrubber*
Item #	$S-301$
Operation	*Continuous*
Type	*Packed Column*
Packing	*INTALOX® saddles ceramic*
Function	
To absorb the H_2S, CO_2 *gas from process Stream*	
Operating Pressure	30 *bar*
Operating Temperature	437.15 °*K*
Diameter	0.786 *m*
Effective Interfacial Area of packing	73.87 (m^2/m^3)
height of an overall gas − phase transfer unit (H_{OG})	0.553 *m*
number of overall gas − phase transfer units (N_{OG})	2.60
Height of Transfer Unit	1.44 *m*
Total Height	3.44 *m*
Pressure drop (ΔP)	0.026 *psi*

CHAPTER # 06

MECHANICAL DESIGN

6. Mechanical design:

Mechanical design of pressure vessels, vessels that are subjected to pressure difference of 0.5 bar, deals with specifying two types of information,

- Vessel wall thickness
- The maximum allowable stress intensity for which the which vessel might be exposed to.

6.1. Mechanical design of water gas shift reactor(R-301):

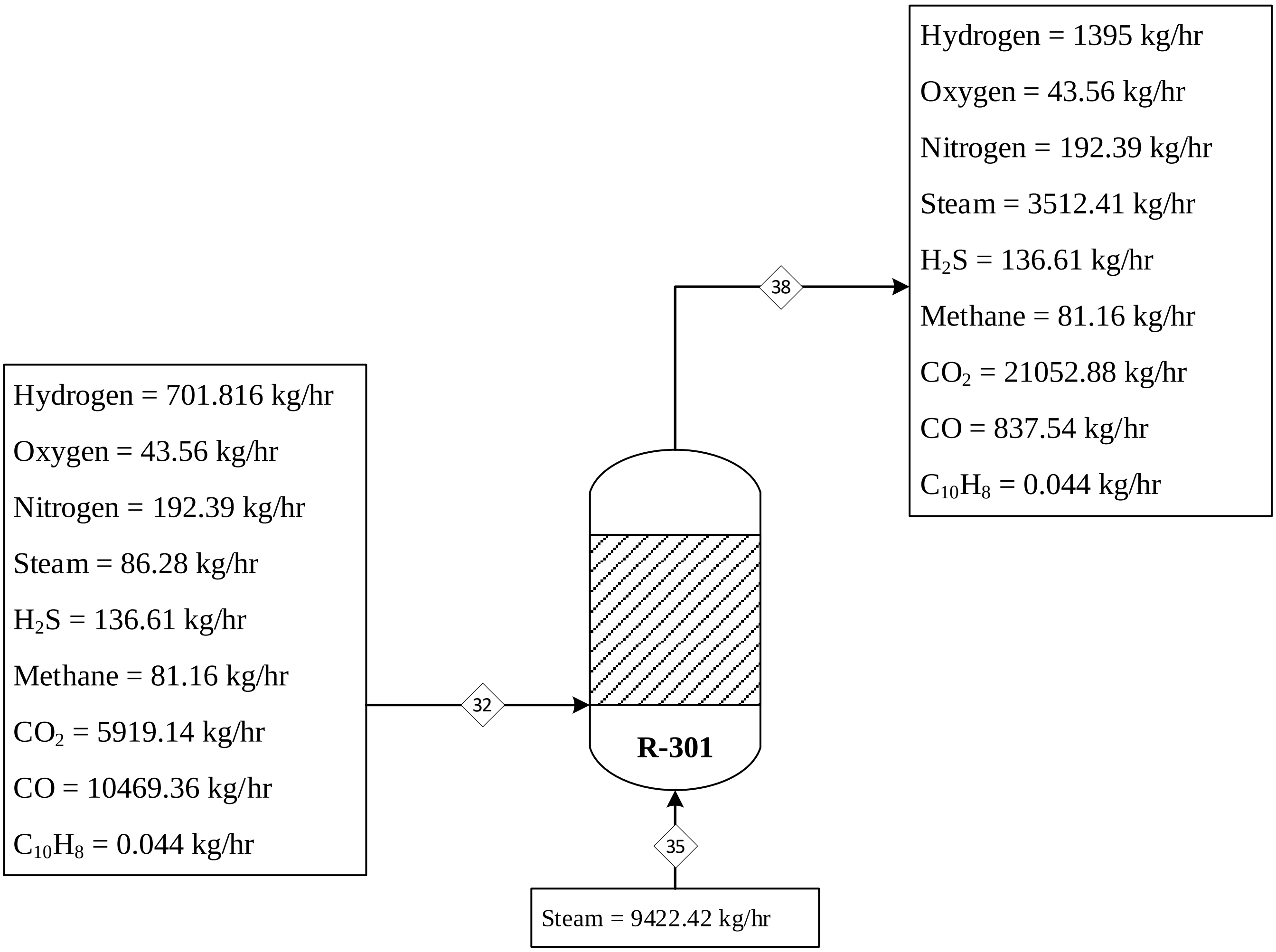


Figure 6.1: *Balance on WGS unit*

$Operating\ temperature\ =\ 350\ {}^0C$

$Operating\ pressure\ =\ 5\ bar$

6.1.1. Design pressure:

- Maximum operating pressure equals 25 psi over operating pressure,

$$= \frac{5\ bar * 14.5\ psi}{1\ bar} + 25\ psi \rightarrow \mathbf{97.5\ psig}$$

- Design pressure is 10% over the maximum operating pressure,

$$= 97.5 + 10\ psi \rightarrow \mathbf{107.5\ psig\ or\ 7.3\ bar}$$

To round off the figure of 7.3 bar to nearest whole number let's say,

$$\mathbf{Design\ pressure\ =\ 8\ bar\ or\ 116\ psig}.$$

6.1.2. Design temperature:

- $Operating\ temperature\ =\ 662\ {}^0F$

The design temperature is taken as 150 ⁰F above than operating temperature because the range given for nominal rule of adding 50 ⁰F doesn't applies here.

$$\boldsymbol{Design\ temperature\ =\ 812\ ^{0}F\ or\ 433^{0}C}$$

6.1.3. Material selection:

$\boldsymbol{Stainless\ steel\ type\ 304\ (Austenitic)}$ fulfills the criteria of selecting as a material of construction in following manner,

- High durability at elevated temperatures and pressures.
- High corrosion resistance is due to the presence of greater concentration of chromium.
- Relatively cheaper than martensitic, ferritic, and duplex type of stainless steel.

6.1.4. Minimum practical wall thickness:

Diameter of reactor $= 1.48$ m or 58.46 inch
Minimum wall thickness is taken as 0.32 inch when diameter lies in the range of $42 - 60$ inches.
Minimum wall thickness $=$ 0.32 inches or 8 mm
For vessel to be rigid enough to bear its own weight its wall thickness must be or greater than 8 mm.

6.1.5. Wall thickness to resist internal pressures:

The thickness to resist internal pressures is given by,

$$t = \frac{P*R}{S-0.6*P} \tag{6.1}$$

Where,
t $=$ Wall thickness (inch)
P $=$ Design pressure (psi)
R $=$ Radius of vessel (inch)
S[48] $=$ Max. allowable tensile stress which is specific for each material (11240.6 psi or 77.5 $\frac{\mathbf{N}}{\mathbf{mm^2}}$)

$$t = \frac{116 * 29.23}{11240.6 - 0.6 * 116} \rightarrow \boldsymbol{0.303\ inch}$$

Corrosion allowance = 0.15 inch

$$Total\ thickness\ of\ the\ shell\ =\ 0.15 + 0.303\ \rightarrow \boldsymbol{0.453\ inch\ or\ 11.43mm}$$

Outer diameter Do $=$ Di $+$ $2 * t$

$$Do = 58.46 + 2 * 0.303 \rightarrow \boldsymbol{59.37\ inch}$$

6.1.6. Selection of head type:

The ends of a cylindrical vessel are closed by heads of various sizes.
The most common forms are;

- Flat plates and formed flat heads
- Hemispherical head
- Ellipsoidal head
- Tori spherical head

The head which gives the minimum thickness under design pressure is selected.

6.1.7. For domed ends,

1) **Tori spherical head**:

$$\boldsymbol{t} = \frac{(0.885\ PL)}{(S-0.1P)} \rightarrow \boldsymbol{0.53\ inch} \tag{6.2}$$

---

[48] Function of temperature and pressure.

Where,

L = crown radius (radius of vessel)

2) **Ellipsoidal head**:

$$\boldsymbol{t} = \frac{PDi}{(2S-0.2P)} \rightarrow \mathbf{0.30}\ \boldsymbol{inch} \tag{6.3}$$

3) **Hemispherical head**:

$$\boldsymbol{t} = \frac{PR}{(2SE-0.2P)} \rightarrow \mathbf{0.15}\ \boldsymbol{inch} \tag{6.4}$$

4) **For Flat ends**,

$$\boldsymbol{t} = Di\sqrt{0.3\frac{P}{S}} \rightarrow \mathbf{3.25}\ \boldsymbol{inch} \tag{6.5}$$

As hemispherical head has minimum thickness under the infliction of design pressure so it would be suitable for selecting head type.

6.1.8. Dead weight of vessel:

The total weight of vessel excluding weight of fittings is known as dead weight and is given by,

$$\boldsymbol{W_v} = 240C_wD_M(H_v + 0.8D_M) * t \tag{6.6}$$

Where,

Wv = Dead weight of vessel

C_w = Factor to account for internal fittings

D_m = Mean diameter of vessel (Di + t ∗ 10 − 3) meters

Hv = Height of vessel (between tangent lines)

t = Vessel wall thickness

$$W_v = 240 * 1.08 * 1.49 * (4.8767 + 0.8 * 1.49) * 11.43$$

$$\mathbf{W_v = 26,933\ N}$$

6.1.9. Weight of external fittings:

Caged ladder = 360 ∗ 6.827 → 2458 N

Platforms for vertical column = 1700 ∗ 35.3 → 60,010 N

Total weight of shell = 26933 + 60010 → **89.4 kN**

- **Type of support**:

i. Saddles support (For horizontal vessels)

ii. Skirt support (For tall vertical columns)

iii. Bracket support (For all type of vessels)

As the height of vessel is not much high so bracket support will be suitable.

6.1.10. Wind loads:

The load per unit length of the column can be obtained via,

$$\boldsymbol{F_W} = P_W + D_{eff} \tag{6.7}$$

where,

Pw = Wind pressure (N/m2)

D_{eff} = Effective column diameter ($D_o + D_o$ × (insulation thickness + t) + 0.4 ∗ 10 − 3)

Typical insulation thickness = 75 mm

$$\mathbf{F_W = 2592\ \frac{N}{m}}$$

6.1.11.Stress calculations of WGS reactor:

Primary and principal stresses are found in order to validate that material type and its thickness are suffici

- **Longitudinal stress**:

The stress which acts along the longitudinal axis of cylindrical vessel and is given by,

$$\boldsymbol{\sigma_h} = \frac{PD_i}{2t} \rightarrow \mathbf{52}\ \frac{\boldsymbol{N}}{\boldsymbol{mm^2}} \tag{6.8}$$

- **Circumferential stress**:

$$\boldsymbol{\sigma_L} = \frac{PD_i}{4t} \rightarrow \mathbf{26}\ \frac{\boldsymbol{N}}{\boldsymbol{mm^2}} \tag{6.9 }$$

- **Dead weight stress**:

The stress due to weight of vessel and its contents along with any other attachments on vessel supports is g

$$\boldsymbol{\sigma_W} = \frac{Wv}{\pi(D_i+t)t} \rightarrow \mathbf{1.66}\ \frac{\boldsymbol{N}}{\boldsymbol{mm^2}} \tag{6.10}$$

- **Bending stress**:

The stress that is causing the vessel to undergo bending is given by,

$$\boldsymbol{\sigma_b} = +\frac{M_x}{l_v}\left(\frac{D_i}{2} + t\right) \tag{6.11}$$

Where,

$\mathbf{M_x}$ = Total bending moment.

$\mathbf{l_v}$ = Second moment area of vessel about the plane of bending.

$$\mathbf{M_x} = \frac{\mathrm{F_w x^2}}{2}$$

Where,

Fw = Wind load per unit length

x = distance from the base of column

$$\mathbf{M_x} = \frac{2592 * (6.82)^2}{2} \rightarrow \mathbf{60,409\ Nm}$$

$$\mathbf{l_v}\ = \frac{\pi}{64}(\mathrm{D_o^4} - \mathrm{D_i^4}) \rightarrow\ \mathbf{0.0078}$$

So, bending stress is,

$$\boldsymbol{\sigma_b} = +\frac{\mathrm{M_x}}{\mathrm{l_v}}\left(\frac{\mathrm{D_i}}{2} + \mathrm{t}\right) \rightarrow \mathbf{5.83}\ \ \frac{\mathbf{N}}{\mathbf{mm^2}}$$

- **Principal stresses**:

The plane that carries the maximum normal stress are called principal plane and the stresses acting on the

$$\boldsymbol{\sigma_1} = \frac{1}{2}\left[\sigma_h + \sigma_z + \sqrt{(\sigma_h - \sigma_z)^2 + 4t^2}\right] \rightarrow \mathbf{52}\ \frac{\boldsymbol{N}}{\boldsymbol{mm^2}} \tag{6.12}$$

Where,

$\boldsymbol{\sigma_z}$ = **Total longitudinal stress** $(\boldsymbol{\sigma_L} + \boldsymbol{\sigma_W} + \boldsymbol{\sigma_b})$

$$\boldsymbol{\sigma_2} = \frac{1}{2}\left[\sigma_h + \sigma_z - \sqrt{(\sigma_h - \sigma_z)^2 + 4t^2}\right] \rightarrow \mathbf{33.4}\frac{\boldsymbol{N}}{\boldsymbol{mm^2}} \tag{6.13}$$

$$\boldsymbol{\sigma_3} = -0.5 \times \mathrm{P} \rightarrow \mathbf{-0.40}\ \frac{\mathbf{N}}{\mathbf{mm^2}}$$

6.1.12. Allowable stress intensity:

The maximum stress intensity at a particular point is taken as the one of the greatest value of following,

$$(\sigma_1 - \sigma_{2)} \rightarrow \mathbf{18.5\ \frac{N}{mm^2}}$$

$$(\sigma_1 - \sigma_3) \rightarrow \mathbf{53\frac{N}{mm^2} < 78\ \frac{N}{mm^2}}$$

$$(\sigma_2 - \sigma_3) \rightarrow \mathbf{34\ \frac{N}{mm^2}}$$

As $(\boldsymbol{\sigma_1 - \sigma_3})$ has highest value so it should not be exceeded than maximum allowable tensile stress (design stress) or else vessel wall thickness or material of construction should be changed.

Table 6.1: *Specification sheet of reactor (R-301)*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	R-301[58]
Operation	Continuous
Type	Multi-tubular fixed bed reactor
Material of construction	Stainless steel-304
Head type	Hemispherical head
Function	
Hydrogen synthesis through water-gas shift reaction	
Design pressure	8 bars
Design temperature	430 ºC
Wall thickness	11 mm
Head thickness	4 mm
Diameter of vessel	1.5 m
Weight of vessel	89 kN
Longitudinal stress	52 N/mm^2
Circumferential stress	26 N/mm^2
Dead weight stress	1.66 N/mm^2
Bending stress	6 N/mm^2
Design stress	78 N/mm^2
Allowable stress intensity	53 N/mm^2

Table 6.2: *Specification sheet of reactor R-302*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	R-302
Operation	Continuous
Type	Multi-tubular fixed bed reactor
Material of construction	Stainless steel-301
Head type	Hemispherical head
Function	
Carbon monoxide synthesis via hydrocarbons reforming	
Design pressure	35 bars
Design temperature	980 ^{o}C
Wall thickness	12 mm
Head thickness	4 mm
Diameter of vessel	0.9 m
Weight of vessel	50 kN
Longitudinal stress	119 N/mm^2
Circumferential stress	60 N/mm^2
Dead weight stress	1.5 N/mm^2
Bending stress	2 N/mm^2
Design stress	172 N/mm^2
Allowable stress intensity	121 N/mm^2

Table 6.3: *Specification sheet of reactor (R-401)*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	R-401
Operation	Continuous
Type	Packed bed reactor
Material of construction	Stainless steel-304
Head type	Hemispherical head
Function	
Hydrogenation of carbon oxides to produce methane	
Design pressure	35 bars
Design temperature	745 ºC
Wall thickness	5 mm
Head thickness	2 mm
Diameter of vessel	0.4 m
Weight of vessel	55 kN
Longitudinal stress	129 N/mm^2
Circumferential stress	65 N/mm^2
Dead weight stress	8 N/mm^2
Bending stress	114 N/mm^2
Design stress	207 N/mm^2
Allowable stress intensity	188 N/mm^2

Table 6.4: *Specification sheet of reactor (R-402)*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	R-402
Operation	Continuous
Type	Packed bed reactor
Material of construction	Stainless steel-304
Head type	Hemispherical head
Function	
Hydrogenation of carbon oxides to produce methane	
Design pressure	35 bars
Design temperature	804 ºC
Wall thickness	5 mm
Head thickness	2 mm
Diameter of vessel	0.4 m
Weight of vessel	51 kN
Longitudinal stress	127 N/mm^2
Circumferential stress	64 N/mm^2
Dead weight stress	8 N/mm^2
Bending stress	115 N/mm^2
Design stress	207 N/mm^2
Allowable stress intensity	189 N/mm^2

Table 6.5: *Specification sheet of reactor (R-403)*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	R-403
Operation	Continuous
Type	Packed bed reactor
Material of construction	Stainless steel-304
Head type	Hemispherical head
Function	
Hydrogenation of carbon oxides to produce methane	
Design pressure	35 bars
Design temperature	702 ^{o}C
Wall thickness	4 mm
Head thickness	1 mm
Diameter of vessel	0.35 m
Weight of vessel	44 kN
Longitudinal stress	148 N/mm^2
Circumferential stress	74 N/mm^2
Dead weight stress	9 N/mm^2
Bending stress	116 N/mm^2
Design stress	281 N/mm^2
Allowable stress intensity	201 N/mm^2

Table 6.6: *Specification sheet of reactor (R-404)*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	R-404
Operation	Continuous
Type	Multi-tubular fixed bed reactor
Material of construction	Stainless steel-304
Head type	Hemispherical head
Function	
Hydrogenation of carbon oxides to produce methane	
Design pressure	35 bars
Design temperature	450 °C
Wall thickness	2.3 mm
Head thickness	0.6 mm
Diameter of vessel	0.3 m
Weight of vessel	33 kN
Longitudinal stress	240 N/mm^2
Circumferential stress	120 N/mm^2
Dead weight stress	15 N/mm^2
Bending stress	130 N/mm^2
Design stress	421 N/mm^2
Allowable stress intensity	266 N/mm^2

Table 6.7: *Specification sheet of reactor (G-201)*

SPECIFICATION SHEET	
Identification	
Item	Reactor
Item no.	G-201
Operation	Continuous
Type	Bubbling fluidized bed gasifier
Material of construction	Stainless steel-304
Head type	Hemispherical head
Function	
Syngas formulation via solid waste gasification	
Design pressure	13 bars
Design temperature	930 ºC
Wall thickness	29 mm
Head thickness	13 mm
Diameter of vessel	2.4 m
Weight of vessel	210 kN
Longitudinal stress	53 N/mm^2
Circumferential stress	27 N/mm^2
Dead weight stress	0.95 N/mm^2
Bending stress	0.6 N/mm^2
Design stress	62 N/mm^2
Allowable stress intensity	54 N/mm^2

CHAPTER # 07

PUMP & COMPRESSOR

7. Compressor:

A compressor is a device that reduces the volume of a compressible fluid (such as air or gas) to raise its pressure. Gas compressors are widely employed in several sectors to transport gas from one tank to another. It is critical to be able to recognize the appropriate sort of equipment based on its individual performance characteristics. The compression stage is simply defined for the process design engineer by the principal purpose of the equipment.

- Reciprocating.
- Centrifugal
- Rotary
- Axial

Compression can occur below atmospheric pressure, as in a vacuum pump, or above atmospheric pressure, as in the majority of process applications. A gas compressor is a mechanical device that lowers the volume of a gas in order to increase its pressure. An air compressor is a machine that compresses air so that it may be used to power other equipment.

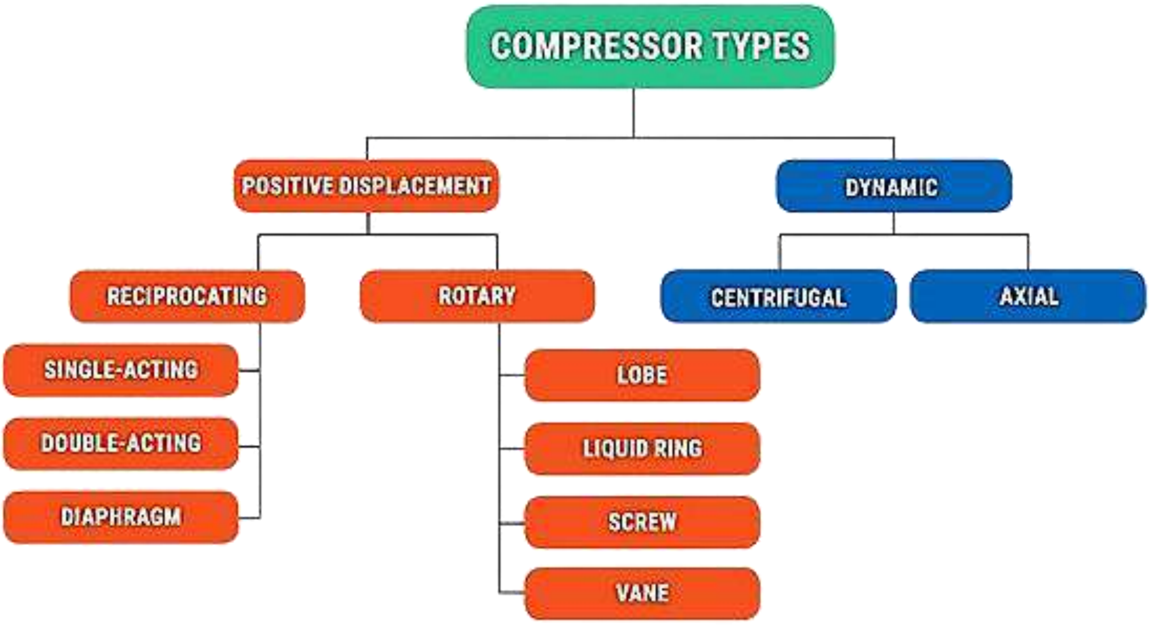


Figure 7.1: *Types of compressors*

7.1. Positive displacement compressors:

- Reciprocating compressor
- Ionic liquid piston type compressors.
- Rotary screw compressors.
- Rotary Vane type compressors.
- Rolling piston compressors

7.2. Dynamic compressor:

- Centrifugal compressor
- Axial compressor
- Diagonal or mixed flow type compressor
- Air bubble compressor

7.3. Design steps for compressor:

1) Calculate volumetric flowrate.

2) Select compressor type.
3) Calculate polytrophic exponent (1st iteration)
4) Calculate discharge temperature.
5) Calculate compressibility functions.
6) Check 1st iteration.
7) Calculate discharge temperature (only if 1st iteration is not satisfied)
8) Again, calculate compressibility functions.
9) Check 2nd iteration and if satisfied.
10) Calculate polytrophic index.
11) Calculate required work done on the gas.
12) Calculate power required.

7.4. Compressor calculations (CO-302):

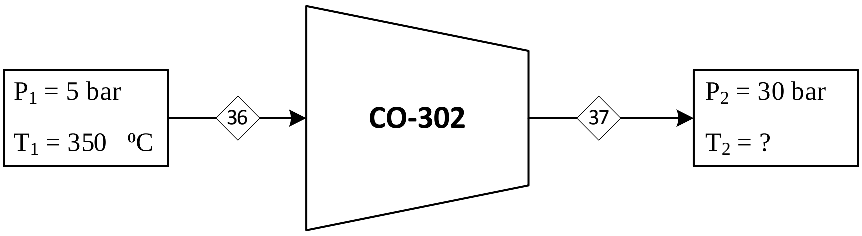


Figure 7.2: *Compressor design.*

Table 7.1: *Component molar flowrate (kmol/hr).*

Component	Molar flow
Hydrogen	691.99
Nitrogen	1.36
Oxygen	6.87
Hydrogen Sulfide	4
Methane	5.06
Carbon dioxide	478.36
Carbon monoxide	29.90
Water vapor	194.97
Naphthalene	0.0003458
Sum	1412.53
Inlet Temperature	350 °C
Outlet Temperature	395 °C
Inlet Pressure	5 bars
Outlet Pressure	30 bars

7.4.1. Volumetric flowrate:

$$Inlet\ volumetric\ flowrate\ = \frac{\dot{n}*22.4*P_o*T_1}{T_o*P_1} \tag{7.1}$$

Where,

$\dot{n} = Inlet\ volumetric\ flowrate$

$P_o = Standard\ pressure$

$T_1 = Inlet\ Temperature$

$T_o = Standard\ Temperature$

$P_1 = Inlet\ Pressure$

Volumetric flowrate is calculated via this formula to compare the expansion volume from ideal conditions.

$$\dot{V} = \frac{\dot{n} * 22.4 * P_o * T_1}{T_o * P_1} \rightarrow \mathbf{14,445}\ \frac{\boldsymbol{m^3}}{\boldsymbol{hr}}$$

7.4.2. Compressor selection:

$$\dot{V} = \mathbf{142}\ \frac{\boldsymbol{ft^3}}{\boldsymbol{sec}}$$

Discharge pressure = 435 psia

From the graph, centrifugal compressor falls under the desired conditions of discharge pressure and volumetric flowrate.

- From graph given below, efficiency of centrifugal compressor is,

$$\boldsymbol{E_P = 0.72}$$

7.4.3. 1st Iteration

7.4.3.1. Calculate polytrophic temperature exponent:

$$m = \frac{\bar{\gamma}-1}{\bar{\gamma}*E_p} \tag{7.2}$$

$Where,$

$\bar{\gamma} = Specific\ heat\ capacity\ ratio\ of\ gaseous\ mixture$

To find specific heat capacity ratio of mixture,

$$\bar{\gamma} - 1 = \frac{\sum_{i=1}^{N} xi}{\sum_{i=1}^{N}(\frac{xi}{\gamma_i-1})} \tag{7.3}$$

$Where,$

$x_i = Mole\ fraction\ of\ each\ component\ in\ gaseous\ mixture$

$\gamma_i = Specific\ heat\ capacity\ ratio\ of\ individual\ gas$

Table 7.2: Mole fraction and specific heat capacity of components

Component	**Mole fraction** (x)	**Specific heat capacity ratio** (γ)
Hydrogen	0.48989	1.405
Nitrogen	0.00096	1.395
Oxygen	0.00486	1.4
Hydrogen Sulfide	0.00284	1.32
Methane	0.00358	1.299
Carbon dioxide	0.33865	1.289
Carbon monoxide	0.02117	1.4
Water vapor	0.13803	1.33
Naphthalene	2.44838E-07	1.03355

So,

$$\boldsymbol{\bar{\gamma} = 1.346}$$
$$\boldsymbol{m = 0.357}$$

7.4.3.2. Calculate discharge temperature:

$$T_2 = T_1 * \left(\frac{P_2}{P_1}\right)^m \tag{7.4}$$

$$\boldsymbol{T_2 = 1182\ K}$$

7.4.3.3. Calculate compressibility functions, X and Y:

- First calculate the pseudo-critical temperature and pressure,

$$\boldsymbol{P_{pc}} = \sum_{i=1}^{N} P_{ci} * x_i \rightarrow \boldsymbol{63.27\ bar}$$

$$\boldsymbol{T_{pc}} = \sum_{i=1}^{N} T_{ci} * x_i \rightarrow \boldsymbol{214\ K}$$

$Where,$
$P_{ci} = Critical\ pressure\ of\ individual\ component$
$T_{ci} = Critical\ temperature\ of\ individual\ component$
Now calculate mean pseudo-reduced temperature and mean pseudo-reduced pressure,

$$\boldsymbol{P_{pr}} = \frac{P_1 + P_2}{2 * P_{pc}} \rightarrow \boldsymbol{0.2765}$$

$$\boldsymbol{T_{pr}} = \frac{T_1 + T_2}{2 * P_{pc}} \rightarrow \boldsymbol{4.21}$$

Heat capacity at mean temperature $= 0.3163\ \frac{\mathbf{KJ}}{\mathbf{mol.K}}$

Now from figure 3.8, 3.9 and 3.10.
$X = 0$
$Y = 1.01$

$Z = 1$

- **Check 1st iteration,**

$$m = \frac{Z*R}{C_p} * \left(\frac{1}{E_p} + X\right) \tag{7.5}$$

$$\boldsymbol{m = 0.0364 \neq 0.35}$$

7.4.4. 2nd Iteration:

7.4.4.1. Calculate discharge temperature:

Calculate T_2 from polytrophic temperature exponent calculated above,

$$\boldsymbol{T_2} = T_1 * \left(\frac{P_2}{P_1}\right)^m \rightarrow \boldsymbol{665.24\ K}$$

7.4.4.2. Calculate compressibility functions:

$$\boldsymbol{P_{pc}} = \sum_{i=1}^{N} P_{ci} * x_i \rightarrow \boldsymbol{63.27\ bar}$$

$$\boldsymbol{T_{pc}} = \sum_{i=1}^{N} T_{ci} * x_i \rightarrow \boldsymbol{214\ K}$$

$$\boldsymbol{P_{pr}} = \frac{P_1 + P_2}{2 * P_{pc}} \rightarrow \boldsymbol{0.276}$$

$$\boldsymbol{T_{pr}} = \frac{T_1 + T_2}{2 * P_{pc}} \rightarrow \boldsymbol{3}$$

Heat capacity at mean temperature $= 0.2944\ \frac{\mathbf{KJ}}{\mathbf{mol.K}}$

X = 0
Y = 1.02
Z = 1

- **Now check 2nd iteration,**

$$m = \frac{Z * R}{C_p} * \left(\frac{1}{E_p} + X\right)$$

$$\boldsymbol{m = 0.0392\ \approx 0.364}$$

7.4.5. Calculate polytrophic index:

$$\boldsymbol{n} = \frac{\mathbf{1}}{\mathbf{1} - \boldsymbol{m}} \rightarrow \boldsymbol{1.04}$$

7.4.6. Calculate required work done:

$$W = \frac{Z*R*T_1*n}{n-1}\left[\left(\frac{P_2}{P_1}\right)^{(n-1)/n} - 1\right] \tag{7.6}$$

$$W = \frac{1 * 0.008314 * 623.15 * 1.0408}{1.0408 - 1}\left[\left(\frac{30}{5}\right)^{(1.0408-1)/1.0408} - 1\right]$$

$$\boldsymbol{W = 9.61\ \frac{kJ}{mol}}$$

7.4.7. Calculate power required:

$$Actual\ work\ done\ =\ \boldsymbol{W/E_p} \qquad (7.7)$$

$$\text{Actual work done} = \left(\frac{\mathbf{9.61}}{\mathbf{0.72}}\right) * \mathbf{1000} \rightarrow \mathbf{13,357}\ \frac{\boldsymbol{kJ}}{\boldsymbol{kmol}}$$

$$Power\ required\ =\ Actual\ work\ done * Molar\ flowrate$$

$$\boldsymbol{P} = \frac{13357 * 1413}{3600} \rightarrow \mathbf{5241}\ \boldsymbol{kW}$$

$$\boldsymbol{Power\ required\ =\ 7028\ hp}$$

- Now calculate the outlet temperature based on polytrophic exponent from 2nd iteration (satisfied).

$$\boldsymbol{T_2} = T_1 * \left(\frac{P_2}{P_1}\right)^m \rightarrow \mathbf{668.5}\ \boldsymbol{K} \qquad \textbf{(7.8)}$$

Table 7.3: *Specification sheet of compressor (C-302)*

SPECIFICATION SHEET	
Identification	
Item	Compressor
Item no.	CO-302
Type	Centrifugal
Function	
To increase pressure of gaseous mixture from 5 to 30 bars	
Feed flowrate	8502 scfm
Inlet pressure	5 bars
Discharge pressure	30 bars
Power	7028hp

Table 7.4: *Specification sheet of compressor (CO-301)*

SPECIFICATION SHEET	
Identification	
Item	Compressor
Item no.	CO-301
Type	Centrifugal
Function	
To increase pressure of gaseous mixture from 10 to 30 bars	
Feed flowrate	3414 scfm
Inlet pressure	10 bars
Discharge pressure	30 bars
Power	3388hp

Table 7.5: *Specification sheet of compressor (CO-201)*

SPECIFICATION SHEET	
Identification	
Item	Compressor
Item no.	CO-201
Type	Reciprocating
Function	
To increase pressure of gas from 1 to 10 bars	
Feed flowrate	96 scfm
Inlet pressure	1 bars
Discharge pressure	10 bars
Power	25hp

CHAPTER # 08

COST ESTIMATION

8. Cost estimation:

Any industrial process need a capital expenditure, and determining the necessary investment is a crucial component of a plant design project. A capital cost estimation for a method may range from a pre-design estimate based on no details other than the planned project's scale to a precise estimate based on full drawings and specifications. Between these two extremes of capital expenditure forecasts, there are a plethora of other estimates that differ in precision based on the project's level of growth. These estimates go by a number of names, but the five groups below reflect the standard precision set and classification for design purposes.

1) Order of magnitude estimates
2) Study estimate (Estimate of the factorial)
3) Preliminary estimates (Estimated Spending Authorization)
4) Definitive estimate (Estimate for project management)
5) Detailed estimate (Estimate from the contractor)

8.1. Cost indexes:

A cost is equivalent to a numerical index value at a certain moment in time that depicts the cost in respect to a base time. As a result, the current cost is calculated using the cost index as follows:

$$\frac{\boldsymbol{Present\ cost\ of\ equipment}}{\boldsymbol{Present\ cost\ index}} = \frac{\boldsymbol{Cost\ of\ equipment\ at\ base\ time}}{\boldsymbol{Cost\ index\ at\ base\ time}}$$

Various types of cost indexes are issued on a daily basis. Others may be used to estimate the cost of machinery, while others are more applicable to labour, manufacturing, supplies, or other specialized areas. The most common of these indices are:

1) Marshal-and-Swift all-industry and process-industry equipment index
2) Engineering News-record construction index
3) Nelson-Farrar construction index
4) Chemical Engineering Plant Cost Index

Chemical engineering plant cost index would be used for estimation of original cost at 2022.

8.2. Capital investment:

It costs a lot of money to buy and install the necessary machinery and equipment before an industrial facility can be put into operation. It is necessary to acquire land, make service facilities available, and construct the plant with all of the necessary pipelines, controls, and services. Additionally, money is needed so that plant operating costs can be paid before sales revenue is made available. It costs a lot of money to buy and install the necessary machinery and equipment before an industrial facility can be put into operation. It is necessary to acquire land, make service facilities available, and construct the plant with all of the necessary pipelines, controls, and services.

Additionally, money is needed so that plant operating costs can be paid before sales revenue is made available. Fixed capital investment (FCI) refers to the funds required to purchase the essential production and plant facilities, whilst working capital (WC) refers to the funds required to operate the plant. Total capital investment (TCI) is the sum of working capital and fixed capital investment.

$$Total\ capital\ investment\ (TCI) = Fixed\ capital\ investment\ + Working\ capital\ investment \qquad (8.1)$$

8.2.1. Fixed capital investment:

Fixed investment is the proportion of a company's total capital expenditure that is committed to acquiring tangible assets such as machines that are utilised indefinitely or for more than one accounting period. The fixed capital is further subdivided into followings,

- Manufacturing fixed capital investment
- Non-manufacturing fixed capital investment.

8.2.1.1. Manufacturing fixed capital investment:

Manufacturing fixed-capital investment refers to expenditures required to install process equipment and purchase all essential parts for seamless process operation. It includes,
Expenses for site preparation,

- Piping,
- Instruments,
- Insulation,
- Foundations, and auxiliary facilities

8.2.1.2. Non-manufacturing fixed capital investment:

The amount required for construction overhead and other plant items that are not directly involved in the process activity is referred to as the non-manufacturing fixed-capital investment. These plant components are as follows:

- Warehouses, labs, and transportation;
- Land
- Processing buildings
- Administrative and other offices
- Shipping, and receiving facilities.
- Utility and waste disposal facilities.

8.2.2. Working capital investment:

Working capital refers to the money needed to keep the plant running. The following items should be considered when calculating working capital,

- Stockpiles of raw materials and equipment
- Semi-finished products in the manufacturing process and finished products in store.
- Receivables (accounts receivable)
- Cash is kept on hand to cover monthly running costs including pensions, bonuses, and raw material acquisitions.
- Accounts receivable
- Taxes to compensate.

8.3. Total cost of equipment in 2022:

8.3.1. Cost of reactor (R-301):

$Diameter\ of\ reactor\ =\ 2\ m$

$Length\ of\ tube\ =\ 4.8\ m$

$Number\ of\ tubs\ =\ 43$

$Heat\ transfer\ area\ =\ 98\ m2$

$Bare\ cost\ of\ reactor\ in\ 2004\ =\$\ 100{,}000$

$Factor\ for\ Pressure\ 1-5\ bar\ =\ 1$

$Type\ factor\ =\ 0.8$

$Material\ factor\ =\ 3$

$$\boldsymbol{Cost\ of\ Equipment\ in\ 2004\ =\ 100{,}000\ \$\ *\ Pressure\ Factor\ *\ Type\ Factor} \qquad (8.2)$$

$Cost\ of\ Equipment\ in\ 2004\ =\ 80{,}000\ \$$

$Cost\ index\ in\ 2004\ =\ 444.2$

$Cost\ index\ in\ 2022\ =\ 808.7$

$$\boldsymbol{Cost\ of\ reactor\ in\ 2022\ =\ Cost\ in\ 2004\ x\ \left(\frac{Cost\ index\ in\ 2022}{Cost\ index\ in\ 2004}\right)} \qquad (8.3)$$

$\boldsymbol{Cost\ of\ reactor\ in\ 2022\ =\ \$\ 145,646}$

8.3.2. Cost of reactor (R-401):

$Weight\ of\ vessel\ =\ 5577\ kg$
$Material\ factor\ =$
$Pressure\ factor\ =$

$$\boldsymbol{Cost\ of\ reactor = 73 \times (W)^{-(0.34)} \times Pressure\ factor \times Material\ factor\ \times W} \tag{8.4}$$

$Cost\ in\ 2022\ =\ \$150,207$
$Cost\ index\ in\ 2004\ =\ 444.2$
$Cost\ index\ in\ 2022\ =\ 808.7$

$$\boldsymbol{Cost\ of\ reactor\ in\ 2022\ =\ \$\ 307,059}$$

8.3.3. Cost of reactor (G-201):

$Weight\ of\ vessel\ =\ 47{,}032\ lb.$
$Diameter\ of\ reactor\ =\ 7.7\ ft$
$Height\ of\ reactor\ (L)\ =\ 15.5\ ft$

$$Cost\ in\ 1985\ =\ F_M * Cb\ +\ Cd \tag{8.5}$$

$$\boldsymbol{Cb\ =\ exp[9.100 - 0.2889 * (lnW)\ +\ 0.04576 * (lnW)^2]}$$
$$\boldsymbol{Cd\ =\ 246 * D^{0.7396} * L^{0.7068}}$$

$\boldsymbol{F_M}\ =\ 1.7$
$Cost\ in\ 1985\ = \$\ 136{,}576$
$Cost\ index\ in\ 1985\ =\ 325.8$
$Cost\ index\ in\ 2022\ =\ 808.7$

$$\boldsymbol{Cost\ of\ reactor\ in\ 2022\ =\ \$\ 339,010}$$

8.3.4. Purchased equipment cost of absorber (S-301):

$Diameter\ of\ vessel\ =\ 1.5\ m$
$Height\ of\ vessel\ =\ 4.2\ m$
$Pressure\ Factor\ 20 - 30\ bar\ =\ 1.4$
$Material\ Factor\ =\ 2$
$Bare\ cost\ of\ vessel\ =\ \$\ 11{,}000$
$Cost\ in\ 2004\ = \$\ 30{,}800$
$Height\ of\ the\ Packing\ =\ 2.1\ m$
$Volume\ of\ packing\ =\ 3.7\ m3$
$Packing\ Material\ =\ 25\ mm\ saddles$
$Cost\ of\ Packing\ Material\ =\ 1400\ \$/m3$

$$\boldsymbol{Total\ Cost\ of\ Packing\ =\ Volume\ of\ packing * 1360\ \$/m3} \tag{8.6}$$

$Total\ Cost\ of\ Packing\ =\ 5193\ \$$

$$Total\ Cost\ in\ 2004\ =\ Cost\ of\ Vessel + Cost\ of\ Packing \tag{8.7}$$

$Total\ Cost\ in\ 2004\ =\ \$\ 30{,}800\ +\ \$\ 5193$
$Total\ Cost\ in\ 2004\ =\ \$\ 35{,}993$
$Cost\ index\ in\ 2004\ =\ 444.2$
$Cost\ index\ in\ 2022\ =\ 808.7$

$$\boldsymbol{Absorber\ cost\ in\ 2022\ =\ \$\ 65,526}$$

8.3.5. Purchased cost of waste heat boiler (WHB-301):

$Heat\ transfer\ area\ =\ 51\ m^2$

$Pressure\ factor\ =\ 1$

$Material\ factor\ =\ 3$

$Fixed\ tube\ sheet\ =\ 0.8$

$U\ tube\ =\ 0.85$

$Kettle\ type\ = 1.3$

$Exchanger\ cost\ =\ \$\ 54{,}000$

$Cost\ in\ 2004\ =\ \$47{,}736$

$Cost\ index\ in\ 2004\ =\ 444.2$

$Cost\ index\ in\ 2022\ =\ 808.7$

$Purchased\ cost\ of\ WHB-301\ in\ 2022\ = \$\ 86{,}907$

8.3.6. Purchased cost compressor (CO-301):

$Type\ =\ Centrifugal\ compressor$

$Power\ requirement\ =$

$$C = 1000 * 6.49 * (hp)^{0.62} \tag{8.8}$$

$Purchased\ cost\ =\ \$\ 1{,}001{,}799.8$

$Cost\ index\ in\ 1985\ =\ 325.8$

$Cost\ index\ in\ 2022\ =\ 808.7$

$$\boldsymbol{Cost\ of\ compressor\ in\ 2022\ =\ \$\ 2{,}486{,}665}$$

Table 8.1:*Total purchased equipment cost*

Total purchased equipment cost	
Equipment's	**Cost**
Reactors	
R-301	$145,646.11
R-302	$127,440.34
R-401	$307,059.39
R-402	$294,470.78
R-403	$266,238.32
R-404	$220,920.92
G-201	$339,010.18
Absorber and Stripper	
S-301	$65,527.59
ST-301	$45,878.52
Waste heat boilers	
WHB-301	$16,268.07
WHB-302	$86,907.03
WHB-303	$19,296.58
WHB-304	$3,600.09

WHB-401	$15,571.53
WHB-402	$13,903.91
WHB-403	$8,607.42
WHB-404	$9,696.17
Heat Exchangers	
HX-201	$2,624.84
HX-202	$5,812.30
HX-401	$61,533.24
Compressors	
CO-201	$36,366.84
CO-301	$2,486,665.34
CO-401	$3,909,400.33
Sum	**$8,488,445.86**

8.4. Estimation of total capital investment:

Table 8.2: *Total capital investment for fluid-solid system*

For fluid-solid system		
Cost type	**Percentage of purchased equipment**	**Cost**
Direct cost		
Equipment Erection (f_1)	0.45	$3,819,800.64
Piping (f_2)	0.45	$3,819,800.64
Instrumentation (f_3)	0.15	$1,273,266.88
Electrical (f_4)	0.1	$848,844.59
Buildings, Process (f_5)	0.1	$848,844.59
Utilities (f_6)	0.45	$3,819,800.64
Storages (f_7)	0.2	$1,697,689.17
Site Development (f_8)	0.05	$424,422.29
Ancillary Buildings (f_9)	0.2	$1,697,689.17
Total physical plant cost (ppc)	**3.15**	**$26,738,604.46**
Indirect Cost		
Design and Engineering (f_{10})	0.25	$6,684,651.12
Contractors Fee (f_{11})	0.05	$1,336,930.22
Contingency (f_{12})	0.1	$2,673,860.45
Fixed Capital ($)	1.4 of PPC	$37,434,046.25
Working Capital ($)	0.15 of FC	$5,615,106.94
Total capital investment ($)		**$43,049,153.19**

So,

$$Total\ capital\ investment\ required\ for\ plant\ =\ \$43\ million$$

8.5. Total production cost:

The third significant component of an economic study is the total cost of operating the plant, selling the items, recouping the capital investment, and contributing to corporate services such as administration and research and development.. These charges are typically grouped together under the umbrella term "total product cost."

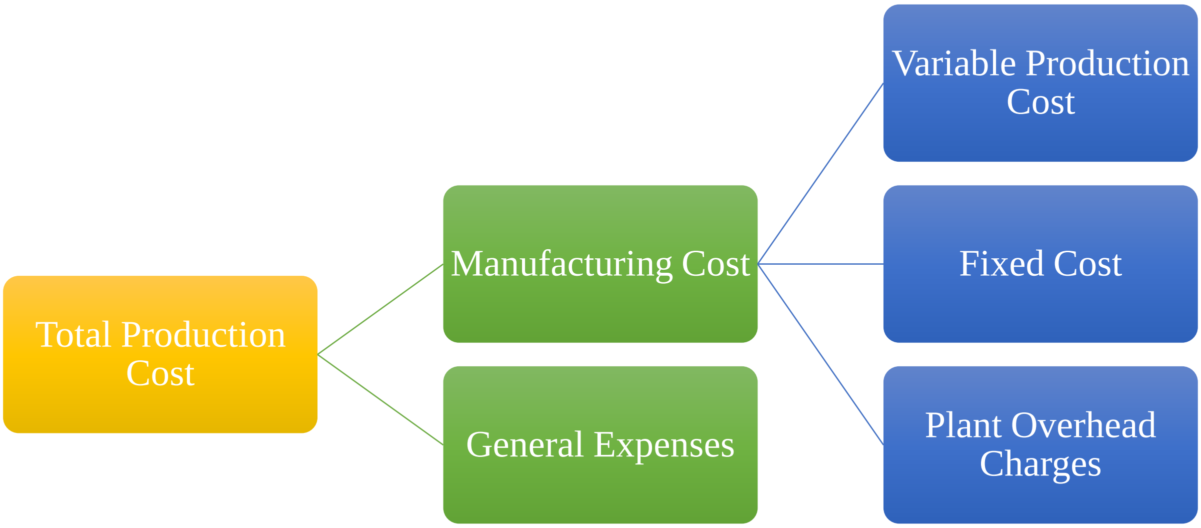


Figure 8.1: *Total production cost*

8.5.1. Manufacturing cost:

Production costs that include any expenses that are directly connected to the production activity or the tangible assets of a process facility. These expenses are sub-divided into,

- Variable Production Cost
- Fixed Cost
- Plant Overhead Charges

8.5.1.1. Variable production cost:

Dynamic production costs include all charges associated with the manufacturing process. This type of cost includes transportation and unloading, direct operating labour, supervisory and clerical labour directly , utilities, plant maintenance and repairs, operating supplies, laboratory supplies, royalties, catalysts, and solvents.

1) Raw material cost:

- $Flowrate\ of\ solid\ waste\ =\ 3.30 \times 10^8\ \frac{kg}{yr}$
- $Price\ of\ solid\ waste\ =\ 0.0103\ \frac{\$}{kg}$
- $Price\ of\ solid\ waste\ per\ year^{49}\ =\ \$\ 3.39\ million$

2) Process steam cost:

- $Flowrate\ of\ process\ steam\ =\ 1.1 \times 10^8\ \frac{kg}{yr}$
- $Price\ of\ steam\ =\ 0.0044\ \frac{\$}{kg}$
- $Price\ of\ steam\ per\ year\ =\ \$\ 0.484\ million$

3) Air from air separating unit:

- $Flowrate\ of\ air\ =\ 7.3 \times 10^6\ \frac{kg}{yr}$

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[49] Plant functioning days are 330.

- $Price\ of\ air\ =\ 0.0051\ \frac{\$}{kg}$
- $Price\ of\ air\ per\ year\ =\ \$\ 37{,}567$

4) Solvent cost:

- $Flowrate\ of\ solvent\ =\ 8.3 \times 10^{7}\ \frac{kg}{yr}$
- $Price\ of\ solvent\ =\ 0.00057\ \frac{\$}{kg}$
- $Price\ of\ solvent\ per\ year\ =\ \$\ 47{,}826$

5) Catalyst cost:

- $Price\ of\ MCR - 2X\ =\ 777.8\ \frac{\$}{864.24kg}$
- $Price\ of\ iron - aluminium\ catalyst\ =\ 1002.06\ \frac{\$}{2004.12kg}$
- $Price\ of\ biomass - char\ catalyst\ =\ \mathbf{8.98}\frac{\$}{\mathbf{57kg}}$

6) Miscellaneous cost:

- $Miscellaneous\ cost\ = 10\%\ of\ maintenance\ cost$[50].
- $Miscellaneous\ cost\ = \$\ 280{,}755$

7) Utilities cost:

→ **Cooling water cost:**

- $Flowrate\ of\ cooling\ water\ =\ 2.2 \times 10^{9}\ \frac{kg}{yr}$
- $Price\ of\ cooling\ water\ =\ 0.00008\ \frac{\$}{kg}$
- $Price\ of\ cooling\ water\ per\ year\ =\ \$\ 179{,}148$

→ **Utility steam:**

- Flowrate of utility steam = $6.5 \times 10^{8}\ \frac{kg}{yr}$
- Price of steam = $0.0044\ \frac{\$}{kg}$
- Price of steam per year = **$ 1.9 million**

$$\boldsymbol{Total\ variable\ production\ cost\ =\ \$\ 6.3\ million}$$

8.5.1.2. Fixed cost:

Fixed expenses are outlays that are unaffected by the rate of output. Depreciation of property taxes, insurance, financing (loan interest), and rent are examples of fixed costs. Except for depreciation, these costs change due to inflation. Because it is controlled by tax regulations, depreciation may vary from year to year, but it is not influenced by inflation.

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[50] Maintenance cost = 7.5% FCI

Figure 8.2: *Fixed cost*

Cost type	Percentages	Cost
Maintenance cost (7.5% of FCI)	0.075	$2,807,553.47
Operating Labor (10% of FCI)	0.1	$3,743,404.63
Laboratory Cost (20-23 % of Operating Labor Cost)	0.215	$804,831.99
Supervision (20% of Operating labor cost)	0.2	$748,680.93
Capital Charges (10% of FCI)	0.1	$3,743,404.63
Insurance (1 % of FCI)	0.01	$374,340.46
Local Taxes (2 % of FCI)	0.02	$748,680.93
Royalties (1% of FCI)	0.01	$374,340.46
Sum		**$13,345,237.49**

$$\boldsymbol{Total\ fixed\ cost\ =\ \$\ 13.3\ million}$$

8.5.1.3. Plant overhead charges:

Plant overhead costs include hospital as well as medical services, general plant maintenance and expenditures, safety services, payroll expenses (including social security and other retirement plans, medical and life insurance, and vacation allowances), packaging, restaurant and outdoor activities, salvage services, control laboratories, safeguarding assets, plant superintendence, warehouse and storage facilities, and special employee benefits. These expenditures are analogous to basic fixed expenses in that they don't fluctuate much with changes in production rate.

$$Plant\ overhead\ charges\ =\ 50\%\ of\ operating\ labour\ cost$$

$$\boldsymbol{Plant\ overhead\ charges\ =\ \$\ 1.8\ million}$$

As,

$$Manufacturing\ cost\ =\ Variable\ Production\ Cost\ +\ Fixed\ Charges\ +\ Plant\ Overhead\ Charges \quad 8.9$$

$$\boldsymbol{Manufacturing\ Cost\ =\ \$\ 21.5\ million}$$

8.5.2. General expenses:

Apart from manufacturing costs, a company's operations entail a variety of general charges. These general expenses may be classified into three categories: administrative costs, distribution and marketing costs, and costs associated with research and development.

Figure 8.3: *General expenses*

General Expenses		
Cost type	**Percentage of manufacturing cost**	**Cost**
Sales Expenses	0.25	$ 5.38 million
General Overheads		
Research and Development		

8.6. Estimation of annual production cost:

Manufacturing Cost = $ 21.5 million + $ 5.38 million
General Expenses = $ 5.38 million

$$\boldsymbol{Annual\ Production\ cost\ =\ \$\,27\ million}$$

- **Annual production rate = $\mathbf{2.20 \times 10^6}$ million British Thermal Units (MMBtu).**

$$Production\ cost\ per\ MMBtu\ = \frac{Annual\ Production\ Cost}{Annaul\ Production\ rate} \qquad (8.10)$$

$$\boldsymbol{Production\ cost\ per\ MMBtu\ =\ \$\,12.25}$$

8.7. Profitability analysis:

Since the purpose of making investments in a chemical plant is to produce money, there must be a system for assessing project economic success. Small projects and basic comparisons of various processing systems and equipment may usually be done by comparing capital and operational expenditures. More complex evaluation methodologies and economic criteria are necessary when picking between large, complicated projects, especially when the projects differ substantially in magnitude, time-frame , and type of product.

8.7.1. Selling price:

$$Market\ price\ of\ RLNG\ = \frac{\boldsymbol{\$15.55}}{\boldsymbol{MMBtu}}$$

$$Selling\ price\ of\ product = \frac{\boldsymbol{\$15}}{\boldsymbol{MMBtu}}$$

$$Gross\ proift\ based\ on\ selling\ price = \frac{\boldsymbol{\$2.75}}{\boldsymbol{MMBtu}}$$

8.7.2. Total income:

$$Annual\ production\ rate\ =\ \boldsymbol{2.20 \times 10^6\ MMBtu}$$

$$Selling\ price\ = \frac{\boldsymbol{\$15}}{\boldsymbol{MMBtu}}$$

$$\boldsymbol{Total\ Income\ =\ \$\,33\ million}$$

8.7.3. Depreciation cost:

For preliminary economic calculations, straight line depreciation method is used.

$Fixed\ capital\ investment\ (V)\ =\ \$\,37.3\ million$

$Salvage\ value$[51] $(Vs)\ =\ \$\,187{,}170.23$

$Recovery\ period\ (N)\ =\ 20$

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[51] Salvage value is 0.5% of FCI

$$\boldsymbol{D = \frac{V-Vs}{N} \rightarrow \$\,1.8\ million} \qquad \textbf{\textit{(8.11)}}$$

8.7.4. Gross profit:

$$Gross\ earnings\ =\ Total\ Income - Total\ Production\ Cost - \ Depreciation\ Cost \qquad (8.12)$$

$$\boldsymbol{Gross\ earnings\ =\ \$\,4.1\ million}$$

8.7.5. Net Income:

$$Net\ income\ =\ Gross\ earnings - \ Gross\ income\ tax \qquad (8.13)$$

Gross income tax = 35% of gross earnings.
Gross income tax = $ 1.4 million

$$\boldsymbol{Net\ profit\ =\ \$\,2.7\ million}$$

8.7.6. Return on investment (ROI):

$$ROI = \frac{Gross\ profit}{Fixed\ Capital\ Investment} \qquad (8.14)$$

$$\boldsymbol{ROI = \ 0.16\ or\ 16\%}$$

8.7.7. Payback period:

$$Payback\ Period = \frac{1}{Return\ on\ investment} \qquad (8.15)$$

$$\boldsymbol{Payback\ period = 6.19 \approx 6\ years}$$

CHAPTER # 09

ISTRUMENTATION & CONTROL

9. Introduction:

Instrumentation is the theory of automated measurement and control. This science has a wide range of applications in modern medicine, business, and everyday life. From automobile engine management systems to house thermostats to aircraft autopilots to prescription medicine production, automation is all around us. This implies, deciding on the optimum measuring technique is an essential initial phase in the design and development of any process control strategy. An operator can read the process variable on a frequent basis and adjust the input up or down to obtain the required temperature in manual operation. Manual oversight is used in uncritical situations when each process shifts states gradually in small increments and requires little supervision from humans. Measurements and changes are done automatically and continuously while under automated control. Because of the following advantages, automated control is still widely used in manufacturing.

- Product consistency is improving, and the pace of output is increasing as well.
- Working conditions are being improved.
- Materials can be saved for less money, and time can be saved.
- Increase safety for personnel and equipment.
- Manual control would not provide for the completion of the process.

9.1. Objectives of instrumentation and control system:

Following are the objectives of Instrumentation and Control System,

1) Reducing external disturbances.
2) Maintaining the process stability.
3) Improve the efficiency of the process.

9.2. Components of a control system:

Following are the components of Control System,

- Process
- Process Variable
- Measuring Element
- Controller
- Final Control Element

1) Process:

Any operation or series of operation that produces a desired final result is a process.

2) Process variable:

The control of process variables is critical to the smooth running of a process. These are characterized as modifications to conditions related to process materials or equipment. Temperature, pressure, flow, and liquid level are the most important factors, followed by a dozen or so less common variables such as chemical composition, viscosity, density, humidity, moisture level, and so on. Measurement is a key requirement for process control, whether it is automated, semiautomatic, or manual. The quality of control obtained is also related to the precision, repeatability, and reliability of the measuring method used.

3) Measuring element:

The measuring element is possibly the most significant of all control system components. If measurements are not taken correctly, the rest of the system will not function properly; also, the measured variable is chosen to reflect the intended circumstances in the process. As a result, choosing the most effective measuring methods is a critical initial step in the design and formulation of any process control system. The four major categories of process deviations are measured, corrected, and modified using an automated control.

i. Temperature measurements
ii. Pressure measurements
iii. Flow rate measurements
iv. Level measurements

Table 9.1: *Various types of measuring instruments for temperature, pressure, flow, and liquid level.*[59]

Measured process variable	Measurement device	Comments
Temperature	• Thermocouples, • Thermometer, thermistor, • Bimetallic Thermometers, • Radiation Pyrometers	• Most common for Relatively Low Temp. • Used for high temp
Pressure	• Manometers • Bourdon tube elements • Bellow elements • Strain gauges • Capsule gauges • Thermal conductivity Gauge • McLeod gauge	• With float or displacers based on the elastics deformation of materials. • Used to convert Pressure to Electrical signal. • For measurement of Vacuum
Flow rate	• Orifice plate • Venture flow nozzle • Dall flow tube • Pitot tube • Turbine flow meter • Hot wire anemometry • Positive displacement • Mass flowmeter	• Measuring pressure drop across a flow Constriction. • Positive displacement and mass flowmeter for high precision.
Liquid level	• Float actuated devices • Displacer devices • Liquid head pressure devices • Dielectric measurement	• Coupled with Various types of indicators and signal converters. • With two phases Indirect method of hydrostatic pressure

9.2.1. Temperature measurement and control:

Temperature measurements are used to regulate the temperature of the output and inlet of process streams. Most temperature measurements in the industry are made using thermocouples to facilitate bringing the measurement to a centralised location for local measurements at the equipment bi-metallic or filled system thermometers are used to a lesser extent usually, high measurements accuracy resistance thermometers are used. When utilised locally, all of these metres are protected by thermo-walls. This protects against the atmosphere and other natural factors.

9.2.2. Pressure measurement and control:

Pressure, like temperature, is a variable that indicates the condition and composition of a substance. In fact, when taken together, these two metrics are the fundamental evaluation devices for industrial materials.

Pressure measurements are extremely important in the reactor. Pressure measurement devices are completed with pumps, compressors, and other process equipment involved with pressure changes in the process material. As a result, pressure measurements might indicate an increase or reduction in energy.

The majority of pressure sensors used in industry are elastic elements devices, either directly linked for local usage or sent to a centralized site. The most common industrial pressure element is a bourdon tube or a diaphragm bellows.

9.2.3. Flow measurement and control:

Flow measurement is an important aspect of practically every industrial process, and numerous methodologies have emerged to do so. Flow measurement often utilizes the same technique as pressure measurement, namely a sensing device connected with a DP cell. Other flow meters may be used for unique situations, such as when there is no external disturbance in the fluid stream, as with magnetic flow meters. Flow indicator controllers are used to manage the volume of liquid; also, all manually configured streams require some flow indication or a simple mechanism for sampling on a regular basis. In industrial, variable head devices are used to measure flow.

9.3. Controller:

The controller is the part of the system that reacts to some error detection system. The controller's output is a fixed property of the defect. The final control factor receives the signal from the controller and changes the energy input to the process based on a predetermined relationship.

9.3.1. Final control element:

A system operated by a controller to adjust the operating conditions of a process is referred to as the final control factor. To work against the mechanism, final control elements require energy. It is the hardware component that carries out the controller's decision.

9.4. Classification of control systems:

For instrumentation and control of different sections and equipment of plants, following control loops are most often used,

- **i.** Feed-back control loop
- **ii.** Feed forward control loop
- **iii.** Ratio control loop
- **iv.** Split range control loop
- **v.** Cascade control loop

9.4.1. Feedback control loop:

A system of control that compares the computed value of a process variable to the intended value of the process variable and takes any necessary actions. Feedback control is the basic structure for control loops. One of its disadvantages is its functioning manner. A monitor will be there to record the value of a quantity entering a process, for example. Any deviations from the set point will be conveyed to the controller, allowing the incoming quantity to be adjusted to the intended value (set point). However, changes have already occurred, and the only thing that can now be done is to implement remedial measures when using feedback.

9.4.2. Feedforward control loop:

The amount of the disturbance is assessed, and action is done to avoid it by changing the quantity of a process variable. This is a control approach for avoiding mistakes in a process variable. This control mechanism is better than feedback control because it predicts the change in the process variable until it reaches the process and takes preventative measures. After a shift occurs in a feedback control system, action is performed.

9.4.3. Ratio control loop:

A control loop that maintains a predefined ratio of one variable to another. This control loop is typically linked to a device in which two distinct systems join a vessel for some form of reaction. This loop ensures appropriate operation in the process vessel by keeping the stoichiometric quantities of various streams constant.

9.4.4. Split range control loop:

This controller has been configured with multiple settings that result in different actions being executed under different scenarios. This loop has the advantage of keeping correct conditions and preventing anomalies at various stages.

9.4.5. Cascade control loop:

By using two or more control loops, the output of one controlling element influences the set point of another controlling element. This control loop is utilized when basic feed forward or feed backward control is insufficient for proper and rapid control. Typically, the first loop is a feedback control loop..

9.4.6. Auctioneering control loop:

This control configuration selectively feds the highest measurement reading to controller and is also known as selective controller, which have one manipulated variable and several measurement outputs.

9.5. Assumptions of preliminary design

The process is grounded on the following categories of assumptions,

9.5.1. Process operability assumptions:

- All the feed available is utilized and the whole product is sellable.
- Oxygen to Feed ratio in the gasifier must be 0.011.
- Range of Cooling water in heat exchangers or other processing facilities is 15-20 ^{o}C.
- The desired SNG product composition is 94% methane.
- Only moisture is removed in the dryer leaving the volatiles inert in the inner structure of solid waste.
- Methanation catalyst can sustain a temperature up to 750 ^{o}C.

9.5.2. Process alternatives:

- Absorption is the most competitive and economical way of removing acid gases.
- Pyrolysis and incineration, relative to gasification, cannot be considered as an alternative for decomposing solid waste because of its lower gas yield and toxic environmental impacts.
- Naphthalene tar reformer is considered a suitable alternative to oil absorption due to the diversification of tar families formed in the gasifier unit.
- A hydro cyclone is required to remove the excess moisture from the SNG.
- Ash from the gasifier is removed via cyclone separator instead of ESP due to the larger size of particles.

9.5.3. Process optimization:

- Conversion of CO & CO_2 in methanation unit is maintained at 99 & 98% via adiabatic cooling.
- Solvent flow rate is 1.8875 of acid gases.
- All the excess heat is utilized in waste heat boilers (product coolers).
- The composition of CH_4 in SNG should not be greater than 94 moles % due to economic concerns.
- Of the CO_2 produced in the water gas shift reactor, only 67% is absorbed by solvent for conserving the methanation ratio.
- Higher pressure methanation is preferred due to unbalanced reaction stoichiometry.

9.6. Description of plant

The thermochemical pathway utilizes gasification technology and subsequent gas cleaning and methanation for producing synthetic natural gas. The short description of the project is as follows,

- Solid waste is indirectly dried via superheated steam to remove excess moisture and the dried solid waste is forwarded to producing methane from the hydrogenation of carbon oxides. Torrefaction unit whereby volatiles are eliminated, making the solid waste more energy dense for gasification.
- The torrefied solid is gasified in the presence of steam and oxygen to undergo various oxidation, and reduction reactions. From the mass balance and energy balance, it is specified that ratio of oxygen to steam is 0.011 and the overall energy pattern follows an exothermic effect.
- The syngas from the gasifier is passed via a tar reformer, for converting naphthalene into CO & H_2, a water-gas shift reactor, for converting CO into CO_2 and H_2, and an absorber for removal of acid gases. To maintain the desired methanation ratio, only 67% of the CO_2 produced in the water-gas shift reactor is absorbed. [60]
- The treated syngas is passed through a series of adiabatic fixed bed reactors via inter-stage cooling for converting carbon oxides into methane. The energy pattern follows an extremely exothermic effect which is removed via an inter-stage product cooler.
- SNG produced via methanation contains excess moisture as a by-product that is removed by first cooling the SNG to the dew point and then separating SNG from moisture via hydro-cyclone.

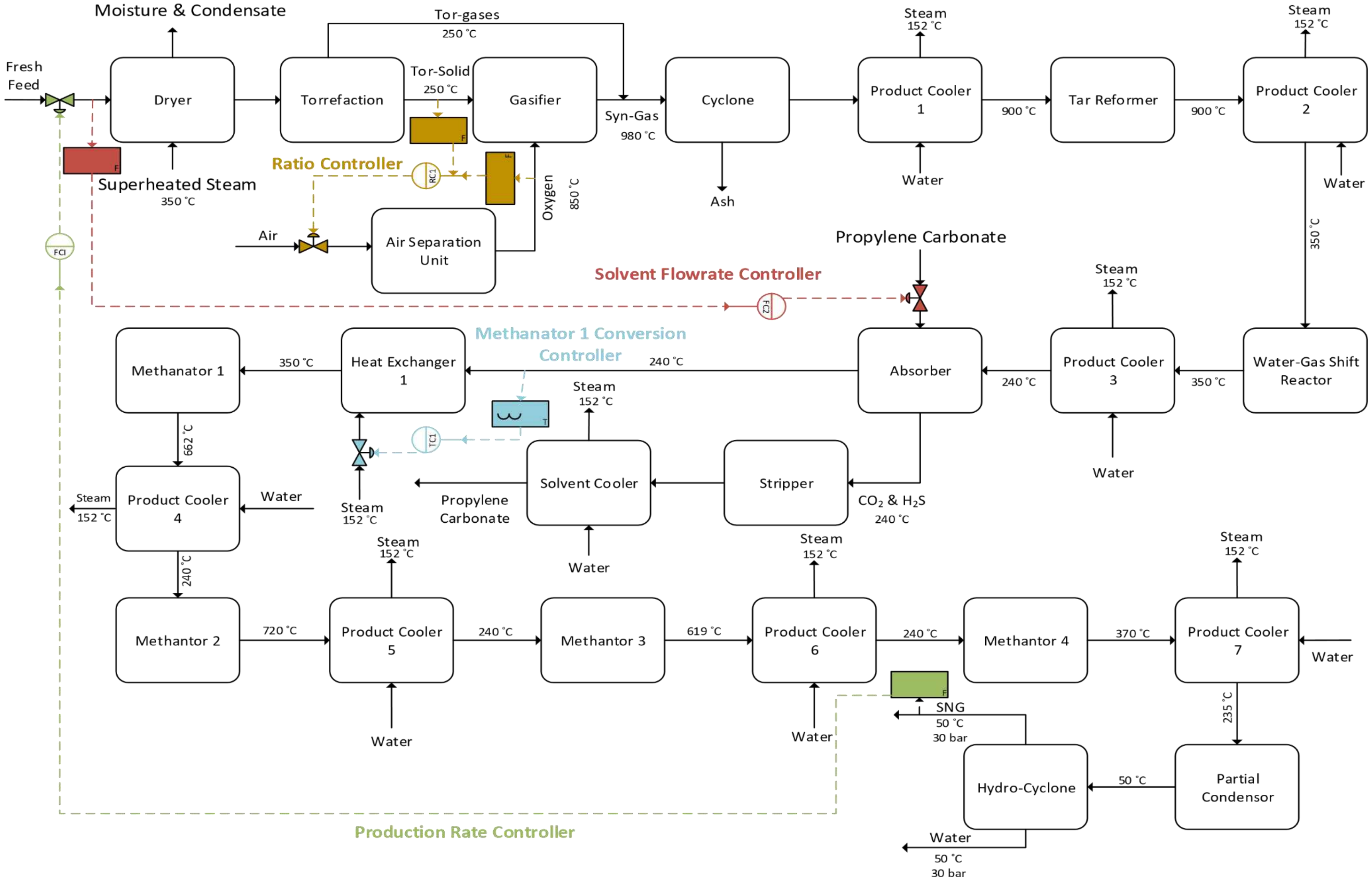


Figure 9.1: *Material balance control on plant.*

9.7. For controlling the production rate:

An increase in the production rate can be done via two manipulated variables,

- Either increasing the conversion of gasifier via increasing temperature leads to a greater amount of syngas but concomitantly reaching ash melting point and causing operability problems. Moreover, an increase in conversion via temperature causes the utility section to produce steam of higher duty which leads to the manipulation of thermal duty of boiler. Applying a controlling mechanism for this method seems unsatisfactory because of higher operating costs and resulting operability issues.
- Or by increasing the feed flow rate by a proportional amount that is required for a production increase. The resulting increment in production cause only a one-time capital investment but reduces the operability problems and makes the control action simple. Therefore, the **feed flow rate is set as a manipulated variable** under constant conversion to control the production rate.

9.8. Material balance control for SNG synthesis plant:

When fresh feed flowrate is changed then the following stream flowrate must change proportionally, [61]

- Oxygen from air separating unit (due to greater amount of oxygen required for oxidation reactions in gasifier).
- Solvent flowrate (A higher amount of propylene carbonate is required to absorb the acid gases up to the desired level set by the methanation unit).
- Water stream flowrates in all the product coolers to produce the steam of required condition. (This is due to the larger the amount of raw material, the greater the temperature rise in the reactor)

9.8.1. Production rate controller:

If the production rate is to be increased or decreased, then the flow rate of the fresh feed should be counted as a manipulated variable because of relative ease in control action. The relation between fresh feed and production rate is as follows,

$$Fresh\ feed = \frac{Production\ rate}{0.0774} \tag{9.1}$$

9.8.2. Ratio controller:

The oxygen-to-feed ratio in the gasifier should be maintained at 0.011 (i.e., mass of oxygen/mass of gasifier feed). An increase in production rate leads to a greater amount of fresh feed which would require more oxygen from ASU for maintaining the desired ratio. If the ratio is disturbed, then required conversions cannot occur in the gasifier so **ratio control** would be suitable to maintain the desired ratio.

$$Oxygen\ from\ ASU\ = 0.011 \times Gasifier\ feed \tag{9.2}$$

9.8.3. Methanator 1 conversion controller:

Conversion of the methanation reactor is a function of temperature and as a result of higher feed temperature, the product stream temperature would be greater than the maximum allowable due to increased conversion. Therefore, to control the temperature and composition of the product stream, the feed temperature should be adjusted via a **feed-forward controller** over the heat exchanger.

9.8.4. Solvent flowrate controller:

Flowrate of the absorber solvent should be adjusted proportionally to increase in production rate and the fresh feed rate. A higher quantity of fresh feed would produce a greater amount of acid gases (i.e. CO_2 & H_2S) which would subsequently require a larger quantity of solvent to have the desired removal of acid gases. So, a **feedforward controller** is employed to predict the solvent flow rate that would be necessary for the purification of syngas in case of an enhanced production rate. Following relationships are devised,

I. $Acid\ gases = 0.1315 * Fresh\ feed$

II. $Solvent\ required = 1.8875 * Acid\ gases$

III. $Solvent\ required = 0.2482 * Fresh\ feed$

Table 9.2: *Summary of material balance controllers for SNG synthesis plant*

Controller	Action
FC1	Controls production rate via manipulating fresh feed flowrate
FC2	Adjust the solvent flow rate as a result of increased/decreased capacity due to variation in production rate.
RC1	Maintains the fixed ratio of one reactant to another for desired conversions in the case of enhanced production rate.
TC1	Maintains the temperature of reactor feed to 350 ^{0}C via utility flow rate in case of varying production rate.

9.9. Product quality control for SNG synthesis plant:

As material balance control is only designed to account for variations in the production rate ordered by top management, there is some space/gap left for controlling or maintaining the constant values of some variables against changes in various disturbances. These variables include product quality or final stream composition. So, a part of the control system that is concerned with the quality of the product delivered is known as product quality control. In SNG synthesis plant product quality control can be accomplished by,

- Regulating the conversion of the reactors will yield lesser composition of undesired components in the final stream.
- Moreover, the effect of substances that remains inert in the reactor and dilutes the final stream should be canceled out via related unit operations (i.e. Physical Absorption).

9.9.1. Control of water-gas shift reactor for ensuring product quality:

To get the desired product quality, conversion in the reactor needs to be maintained by controlling the temperature of the feed stream. If by any means, the quality of the product stream in terms of the desired component is to be increased then there are two pathways for increased conversion,

- Either increase the temperature of the feed stream via the heat exchanger that is located upstream of the reactor.
- Or by increasing the utility stream (in the jacket) temperature that results in reactor temperature rise.

The first approach is suitable because it allows the control action to be implemented earlier.

Table 9.3: *Possible control loop configurations*

Configuration Number	**Control of Composition of Product Stream**	**Control of Reactor Outlet Temperature**	**Comments**
1	Steam Flowrate	Steam flowrate	(1)
2	Utility (in the jacket) flowrate	Utility stream flowrate	(2)
3	Increased/Decreased Packing Height	Steam flowrate	(3)

i. A rapid response from the controller.

ii. Relatively slower response because control action is implemented after the feed has entered the reactor.

iii. Control of composition is not necessarily done by varying packing height due to an increase in operating cost.

Configuration (1) is considered the best due to,

- An increased efficacy of control action by implementing the control output before the feed enters the reactor.
- Steam flow rate also has an impact on the reactor outlet temperature due to controlling action implemented on feed temperature to avoid maximum temperature rise in the reactor.

In the control loop shown, the composition of the desired component in the product stream needs to be increased by increasing the temperature of reactor feed via the steam flow rate. The control action is implemented via a cascade loop that combines the action of the composition controller (master loop) and steam flowrate controller (slave loop). The composition controller calls for an increased temperature, due to the required composition in the product stream, and sends a primary signal to the temperature controller. At the same time, the temperature controller receives another signal from the temperature transmitter of the utility stream and allows the regulation of the valve to adjust the steam flow rate as per the composition required in the product stream and the maximum allowable temperature of the reactor feed.

Cascade Control Loop on Water-Gas Shift Reactor

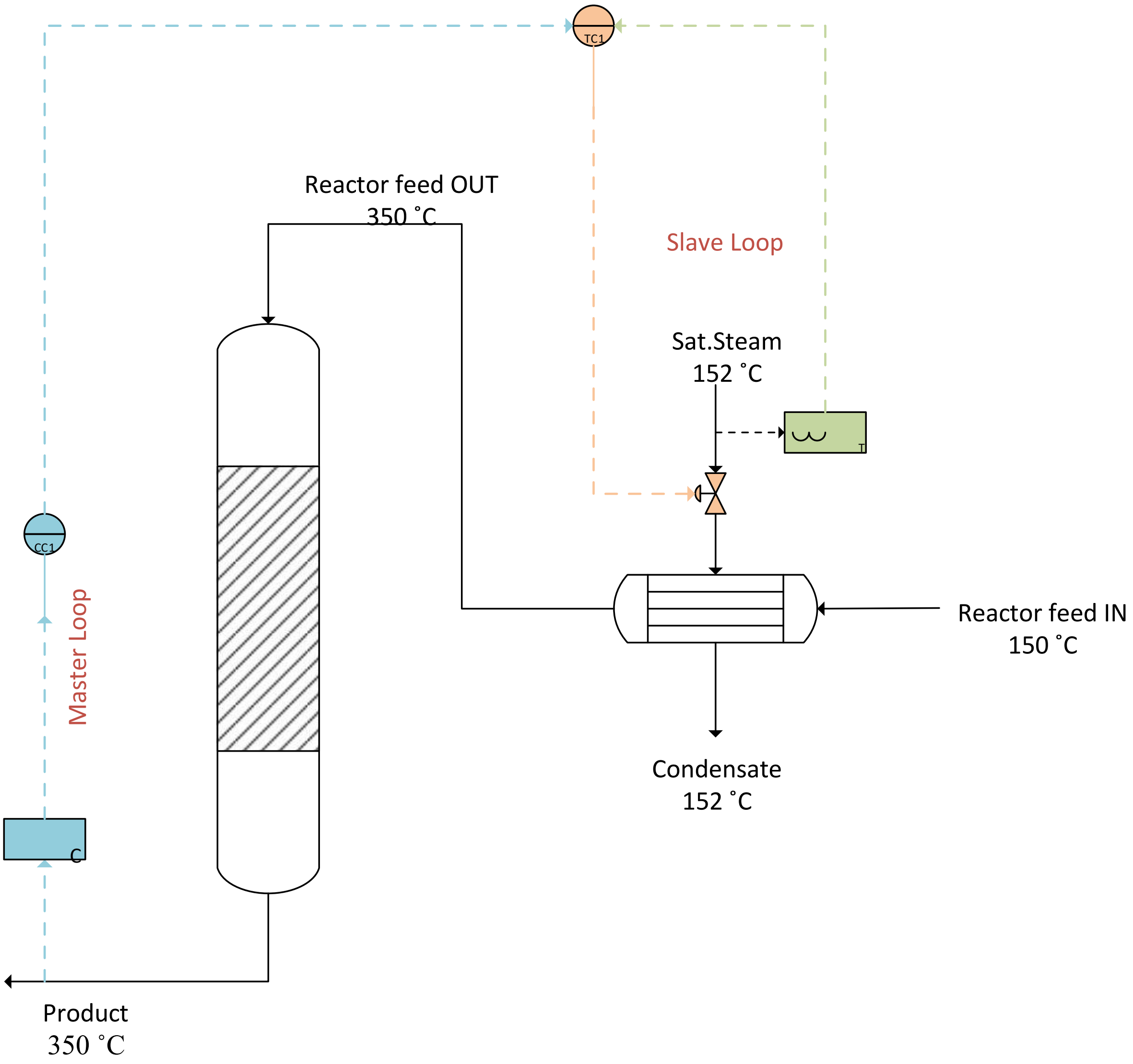


Figure 9.2: *Cascade control loop on water-gas shift reactor*

9.9.2. Control action on absorber for ensuring product quality:

The raw synthesis gas contains acid gases that need to be removed for guaranteeing the proper functioning of downstream equipment. In case of any fluctuations in the production rate, there is a quantitative increase in the acid gases which would require a proportional increase in solvent flow rate for maintaining the syngas quality.

- Have relative ease in control action and height control.
- Decreased production rate due to reduced gas flowrate.
- Longer response time in temperature control,
- Complex and longer response time in terms of height control and treated solvent.

For maintaining the product quality, following are the configurations,

Configuration Number	**Product Quality**	**P Control by**	**T Control by**	**H Control by**	**Comments**
1	Solvent Flowrate	Treated Syngas	Raw Syngas	Lean Solvent	(1)
2	Reduced raw gas flowrate	Rich Solvent	Lean Solvent	Rich Solvent	(2)
3	Substitute Solvent	Raw Syngas	Treated Syngas	Raw Syngas	(3)
4	Solvent Flowrate	Lean Solvent	Treated Solvent	Treated Syngas	(4)

Configuration (01) is considered best due to,

- Rapid response time and ease of control action

Feed-forward Control Loop on Absorption Column

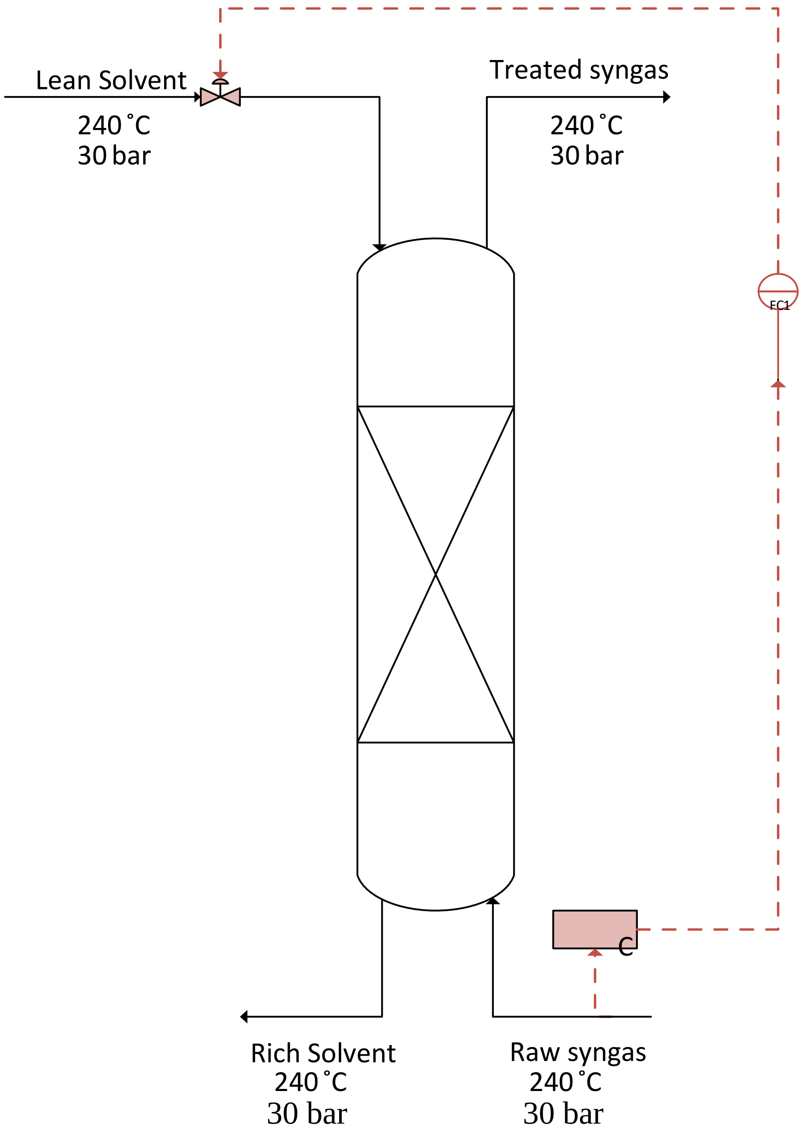


Figure 9.3: Feed-forward control loop on absorption column

The control loop shown works by measuring the concentration of acid gas (in raw syngas) and employing appropriate control action for any adjustment in product quality. If the concentration of acid gases is increased in the raw syngas, due to increased production, then solvent flow rate is increased appropriately, to have desired product quality, by the controller mechanism.

9.10. For maintaining isothermal condition:

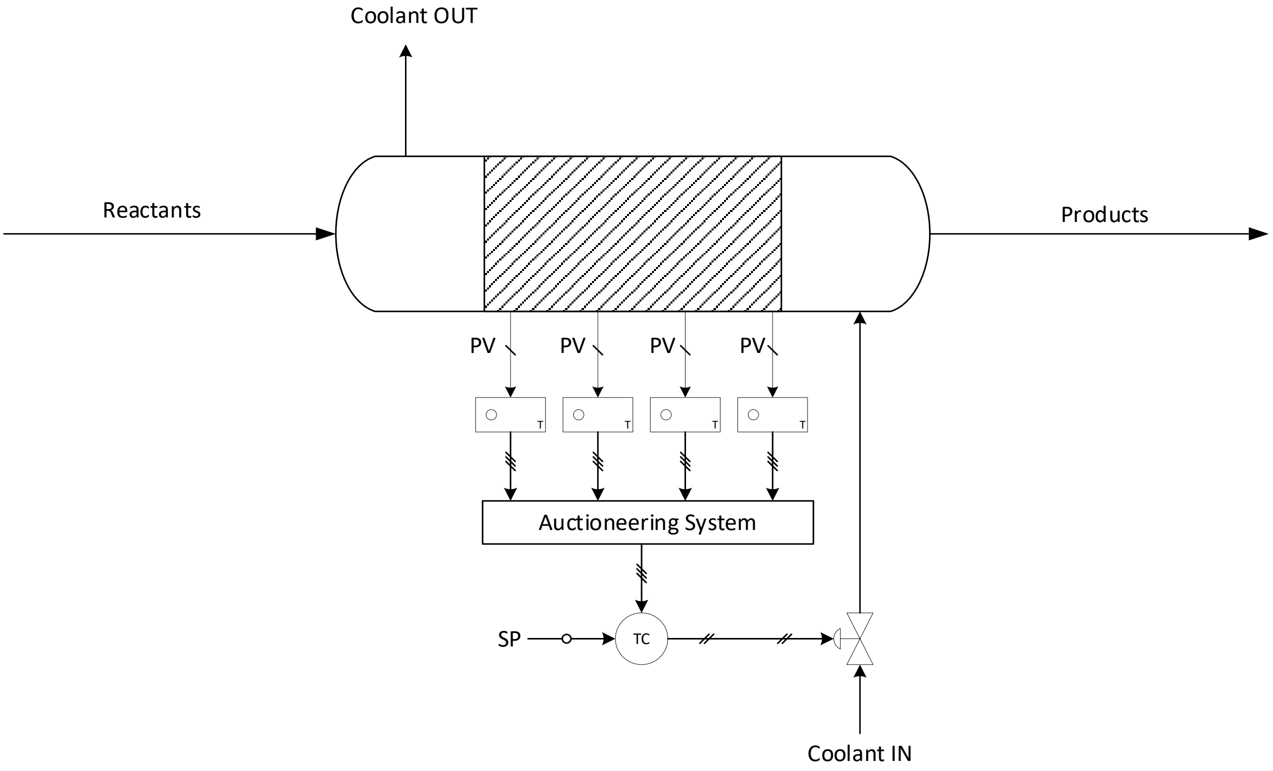


***Figure 9.4:** Control loop scheme of reactor (R-301)*

1) **Objectives:**

Following are the control objectives of reactor (R-301),

- Maintaining isothermal condition inside the reactor by measuring the maximum temperature rise and delivers appropriate coolant flowrate.

2) **Manipulated variable:**

- Coolant flowrate
- Disturbances:
- Feed flowrate.
- Feed concentration.
- Feed temperature.
- Coolant flowrate.
- Coolant temperature.

3) **Auctioneering control system:**

Auctioneering control system measures the process variable on several points along the length of reactor and determines the maximum temperature rise occurring inside the reactor. This maximum temperature rise is the dominant signal sent to controller which manipulates the valve position (vary coolant flowrate) accordingly.

9.11. For controlling process stream temperature:

1) Objectives:

- Maintaining the outlet process stream temperature

2) Manipulated variable:

- Coolant flowrate
- Inlet process stream flowrate
- Disturbances:
- Feed flowrate.
- Feed temperature.
- Coolant flowrate.
- Coolant temperature.

3) Cascade control system:

Consider a heat exchanger in which process stream has to be elevated to temperature of T_2 by using steam as a utility stream having temperature Tc. If there is some disturbance or variation in inlet process stream temperature T_1 then this would have an effect T_2 without regarding any variation in steam flowrate. In order to suppress the effect of disturbance of T_2, steam flowrate should be manipulated in such a way that T_2 remains at given setpoint. Now suppose there is some variation is measured in T_2, this variation is signaled to controller TC_1 which compares it with the given setpoint and generates an error signal to be sent to controller TC_2. This error signal is the setpoint of controller TC_2, which doesn't only adjust the flowrate according to the error signal made by TC_1 but also accounts for any disturbance in steam temperature that would be sufficient to maintain the process variable to desired value.

Cascade control configuration contains multiple closed loop systems of which one loop that measures the process variable is known as primary or master loop, while the second loop that takes the setpoint from primary loop and also accounts for any disturbances in secondary loop is known as slave loop. It consists of two or more than two measurements and only one manipulated variable.[62]

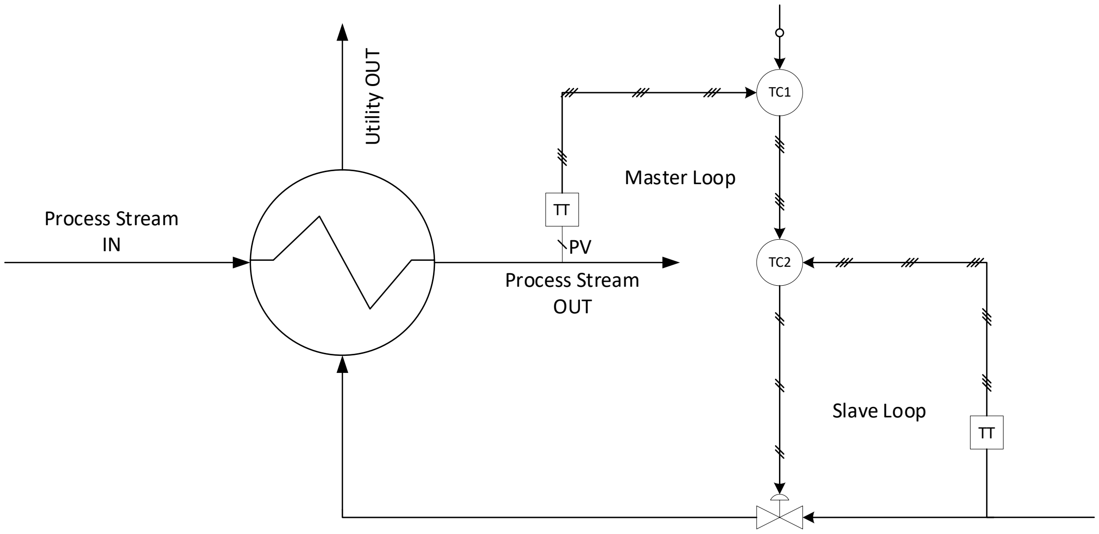


Figure 9.5: *Control loop scheme of heat exchanger*

CHAPTER # 10

HAZARD & OPERABILITY ANANLYSIS

10. Introduction to HAZOP:

A HAZOP study is a systematic process for detecting risks in a chemical plant. The technology detects hazards well and is frequently utilized in the chemical industry. The fundamental premise is to allow the mind to wander in a balanced manner in order to comprehend all of the different ways that process and organizational issues might arise. Specific process knowledge is required before the HAZOP analysis can begin. There are also phase flow diagrams (PFDs), process and instrumentation diagrams (P&IDs), detailed system requirements, design components, and mass and energy balances.

For the comprehensive HAZOP report, a committee comprising of seasoned 'plant, laboratory, technology, and safety practitioners is necessary. One person must be knowledgeable with both the HAZOP protocol and the chemical approach under consideration. Although a variety of vendors offer applications to perform this operation on a personal computer, the responsibility of documenting the data must be assigned to one person. A HAZOP study takes a large amount of time and work, but the relevance of the results is well worth the effort.

A Hazard and Operatability (HAZOP) analysis is a disciplined and methodical assessment of a proposed or current process or operation to detect and assess problems that might endanger persons or equipment or prohibit efficient operation. HAZOP was originally created to analyse chemical process systems, but it has now been expanded to include additional types of systems, as well as complex operations and software systems. A HAZOP is a qualitative technique that is carried out by a group of professionals from various fields (HAZOP team) across a series of sessions.

The HAZOP research should ideally be performed as soon in the design process as feasible in order to have an impact on the design. On the other hand, in order to conduct HAZOP, we need a very comprehensive design. As a compromise, the HAZOP is often performed as a last check after the detailed design is complete. A HAZOP analysis of an existing facility may also be performed to identify adjustments that should be undertaken to mitigate risk and functionality issues.

10.1. Background:

A HAZOP report addresses hazards and operability issues. The concept comprises considering how the plant could react to the design aim. If a solution appears during the process of locating a problem during a HAZOP analysis, it is recorded as part of the HAZOP result; however, caution should be exercised in attempting to locate solutions that are not so obvious, because the primary goal of the HAZOP is to detect problems. While HAZOP research was initially intended to supplement experience-based practice when a new design or technology is involved, it is now used in almost every stage of a plant's life. HAZOP is built on the premise that by bringing together a varied group of specialists, they will cooperate and uncover more issues than if they worked alone then merged their results. The "Guide-word" HAZOP is the most well-known; nonetheless, various specializations of this simple system have arisen.

10.2. Objective of HAZOP study:

The following are the aims of a HAZOP study:

- To recognize (topics of the design that might pose a major risk).
- To identify and investigate design elements that impact the likelihood of a hazardous occurrence occurring.
- To acquaint the research team with the available design data.
- To guarantee that regions of substantial hazard potential are thoroughly studied.
- Identify relevant design details that is not presently accessible to the team.
- To give a method for comprehensive remarks from the research team to the customer.

10.3. HAZOP’s failure or success:

The HAZOP's success or loss is determined by a number of factors:

- The completeness and precision of the drawing and other details that served as the study's foundation.
- The team's ability to visualize deviations, effects, and consequences using the method as a tool to aid their creativity.
- The team's willingness to focus on the more severe risks that have been found.

10.4. Steps to conduct HAZOP study:

A HAZOP study is conducted in the following steps:

I. Outline the study's aim, objective, and context. The goal might be to analyses a yet-to-be-built facility or to assess the risk of an existing unit. The objectives described above might be made more explicit based on the study's aim and conditions. The study's scope includes the physical unit's limits as well as the variety of events and factors evaluated. HAZOPs, for example, were once concentrated mainly on fire and explosion terminals, but now the scope typically includes hazardous release, unpleasant odor, and ecological endpoints.

II. Choose the HAZOP research team. To enable good group interaction, the team leader should be knowledgeable in HAZOP and interpersonal methods. The team should include as many different specialists as possible to cover all elements of design, operation, process chemistry, and safety. The team supervisor should train all members on the HAZOP protocol and underline that the final goal of a HAZOP survey is hazard detection; issue resolution is a distinct activity.

III. Collect data that consists of the following materials,

- A description of the process.
- A flowchart of the process.
- Data on all raw materials, intermediates, and products' chemical, physical, and toxicological qualities.
- Piping and instrument diagrams (P&IDs).
- Specifications for equipment, pipelines, and instruments.
- Logic diagrams for process control.
- Design sketches.
- Policies and procedures.
- Procedures for maintenance.
- Procedures for dealing with emergencies.
- Manuals for safety and training.

IV. Carry out the research. The unit is split into study "nodes" using the information gathered. Nodes are places in the process when process parameters (such as pressure, temperature, and composition) are known and intended. These values vary across nodes due to the functioning of various pieces of equipment, such as distillation columns, heat exchangers, and pumps. Several forms and task sheets have been created to aid in the organization of node process parameters and control logical information.

V. After the nodes and parameters have been identified, every node is investigated through assigning the specialized guiding words to each parameter. These guiding words and their definitions are critical components of the HAZOP method.

VI. The essence of the HAZOP research is repeated cycling through this method, which evaluates how and why each parameter may differ from the planned and the consequences.

VII. Prepare the report. The study should unearth as much detail regarding events and their consequences as possible. Obviously, if the HAZOP indicates a reasonably likely sequence of circumstances that may result in a disaster, adequate follow-up action is required. As a result, while risk reduction activity is not included in HAZOP, it may be required as a result of the HAZOP.

VIII. HAZOP experiments are laborious and expensive. Just updating the P&IDs on an older plant may require a significant technical effort. Still, for processes with significant risk, they are cost effective when balanced against the potential loss of life, property, business, and even the future of the enterprise that may result from a major release.

10.5. Guide words of HAZOP:

Table 10.1: *Guide words of HAZOP*

Guide word	Meaning	Comment
NO, Not, None	Complete negation of the meaning	Nothing more occurs, but no aspect of the design purpose is realized.
More, Higher, Greater	Quantitative increase	Applies to quantities such as flow rate and temperature and to activities such as heating and cooling.
Less, Lower	Quantitative decrease	Applies to quantities such as flow rate and temperature and to activities such as heating and cooling.
As well as	Qualitative increase	All of the concept and operational objectives are met, as well as certain additional activities.
Part of	Qualitative decrease	Just some of the design goals are accomplished while others are not.
Reverse	Opposite of the objective	The opposite of the intention happens. Often applies to activities.
Other than	Complete substitution	The initial goal is replaced by something new when no aspect of it is fulfilled.

10.6. HAZOP study on reactor:

Table 10.2: *HAZOP study on reactors*

Guide word	Process parameter	Possible causes	Possible consequences	Actions required
No	Flowrate	Supply line burst Feed valve is choked	No reaction occurs	Pipe maintenance Valve that operates Automatically
	Pressure	Supply line has leakage.	For variable density systems,	Employ pressure controller

		Excess pressure drops in the pipeline	reaction rate is decreased.	
	Temperature	Malfunctioning of heating media to supply appropriate temperature for reactor.	Decreased product formation	Check utility temperature. Check utility stream pipeline.
More	Flowrate	Failure of feed valve.	Temperature rise in the reactor	Check valves for maintenance
	Pressure	Malfunctioning of compressor.	Leads to more conversion that again further leads to rise in temperature.	Install pressure relief valves.
	Temperature	Malfunctioning of heating media to supply appropriate temperature for reactor	Appropriate conversion may not be achieved.	Check utility temperature. Install temperature indicators.
Less	Flowrate	Supply line rupture Feed valve failure	Less production.	Automation. Maintenance activities.
	Pressure	Leakage in supply line	For variable density systems, reaction rate is decreased.	Employ pressure controller.
	Temperature	Malfunctioning of heating media to supply appropriate temperature for reactor.	Appropriate conversion may not be achieved.	Check utility temperature. Check utility stream pipeline
As well as	Impurities in the feed stream	Failure to remove impurities up to desired extent by upstream equipment.	Decreased yield in product. May promote side reactions. Catalyst deactivation	Ensure purification/conditioning section works within required limits.
Part of	High percentage of reactant A with respect to reactant B.	Inappropriate stoichiometric ratios.	Effect on yield of product.	Employ ratio control loop.

Reverse	Chemical deactivation of catalyst.	Inappropriate reactor temperature may promote reaction between catalyst and one of the reactants.	Catalysts active sites gets occupied. Reaction rate is decreased. Desired product yield is lowered.	Use automatic temperature controllers to avoid the lower limit for temperature inside the reactor.
Other than	Replacement of key reactant with some other component.	Inappropriate study of the reaction mechanism.	Undesired reaction. May poison the catalyst.	Enhance understanding of the reaction mechanism.

CHAPTER # 11

PROCESS SIMULATION & MODELLING

11. Aspen Plus:

ASPEN is an abbreviation for Advanced System for Process Engineering. It is based on a flowsheet simulation. A flowsheet simulation is a type of software used to quantitatively represent a chemical processing facility, including pre- and post-treatment stages as well as the core reactor unit. In the simulation of a full chemical process, each icon represents a unit operation, chemical phase, input/output material source, input/output energy stream, or input/output electric/pneumatic signal, beginning with the raw material and ending with the final finished product.

Using a flowsheet simulator such as Aspen Plus, we may mimic the 11operations of a process using basic engineering relationships. A lot of variables contribute to the creation of such a relationship:

- Equilibrium equations for a wide range of thermodynamic properties, including mass, mole, and energy.
- Phase and chemical equilibrium thermodynamic relationships for reacting and non-reacting media.
- Momentum, heat, and mass transfer rate correlations.
- Stoichiometry and kinetic data for the reaction.

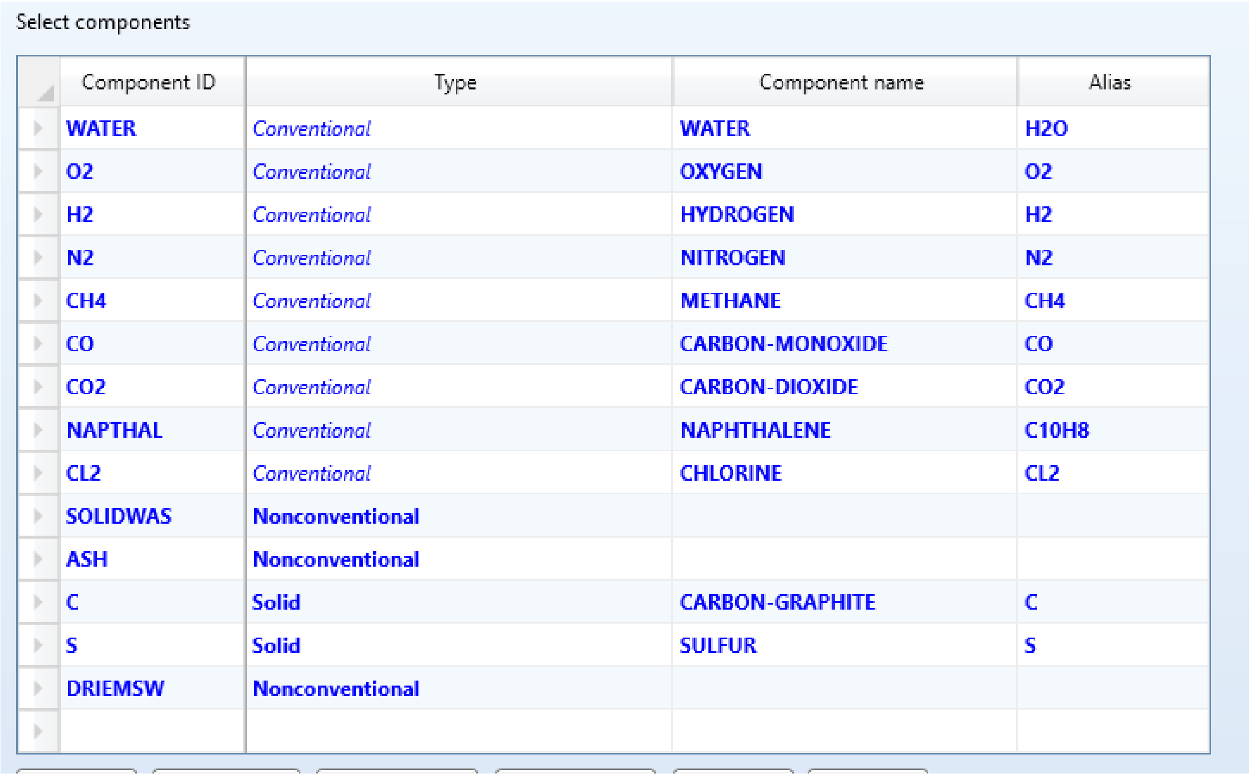
11.1. Process simulation modal for Aspen Plus:

In general, a chemical system is composed of chemical components or distinct organisms that are exposed to physical, chemical, or combined treatments. The skeleton stages listed below can be utilized to transform a process into an Aspen Plus process simulation model.

1) Specify the chemical components that will be used in the process. These components can be retrieved from Aspen Plus databanks or added to the Aspen Plus platform.
2) Develop thermodynamic models to represent the physical properties of the process's components and mixtures. Aspen Plus comes with these models pre-installed.
3) Create a Flowsheet for the process:
    - Define the process's unit operations.
    - Identify the process streams that enter and exit the device operations.
    - To explain each unit procedure or chemical synthesis, select models from the Aspen Plus Model Library and position them on the process flowsheet.
    - As part of the process flowsheet, mark each unit operation model (i.e., block) and join the blocks using process streams.
4) For each feed source, specify the component flow rates as well as the thermodynamic specifications (temperature, pressure, and composition).
5) Define the unit operation models' operating parameters (i.e., blocks).

11.1.1. Components:

The total components that are involved in the synthesis of SNG are,



Select components

Component ID	Type	Component name	Alias
WATER	Conventional	WATER	H2O
O2	Conventional	OXYGEN	O2
H2	Conventional	HYDROGEN	H2
N2	Conventional	NITROGEN	N2
CH4	Conventional	METHANE	CH4
CO	Conventional	CARBON-MONOXIDE	CO
CO2	Conventional	CARBON-DIOXIDE	CO2
NAPTHAL	Conventional	NAPHTHALENE	C10H8
CL2	Conventional	CHLORINE	CL2
SOLIDWAS	Nonconventional		
ASH	Nonconventional		
C	Solid	CARBON-GRAPHITE	C
S	Solid	SULFUR	S
DRIEMSW	Nonconventional		

Figure 11.1: *Selection of input component*

11.1.2. Property method/package:

"A collection of models used to quantify thermodynamic, kinetic, and transport properties is referred to as a property method".

The following Hierarchy is used in the selection of the Property Package,

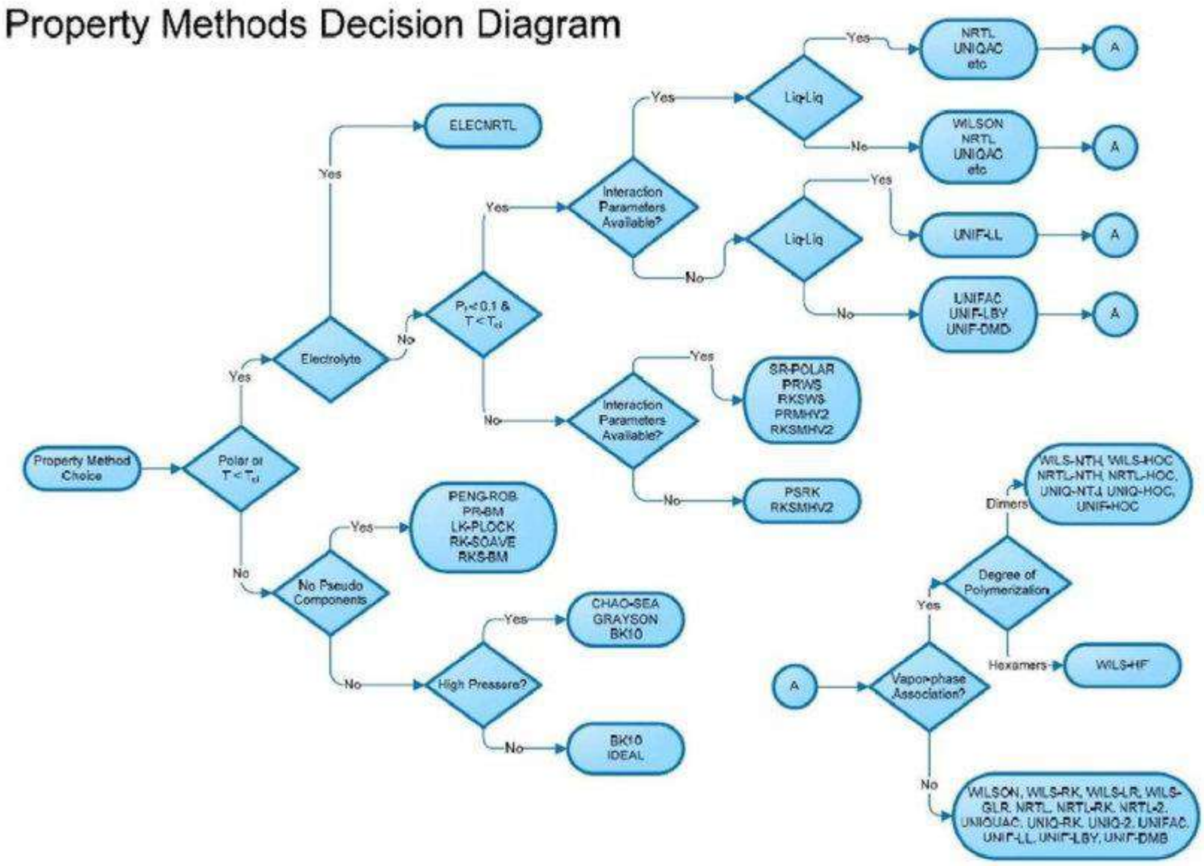
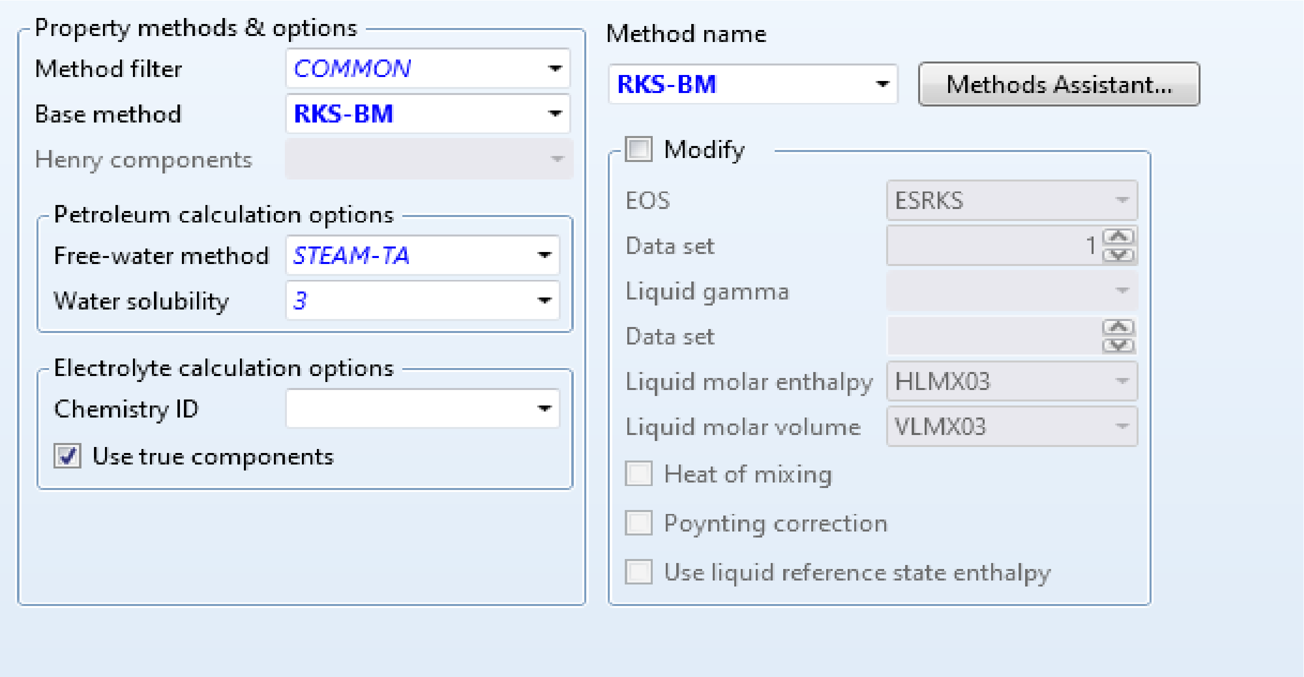


Figure 11.2: *Hierarchy of property method used Aspen Plus*

RKS-BM is selected as the property package by looking at a number of factors, such as:

- The chemical components used in the system are mostly non-polar.
- Binary inputs being available.
- Handling a non-liquid-liquid system.
- Vapor Phase Association



Property methods & options

Method filter: COMMON

Base method: RKS-BM

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Method name: RKS-BM

☐ Modify

EOS: ESRKS

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX03

Liquid molar volume: VLMX03

☐ Heat of mixing

☐ Poynting correction

☐ Use liquid reference state enthalpy

Figure 11.3: *Selecting property method.*

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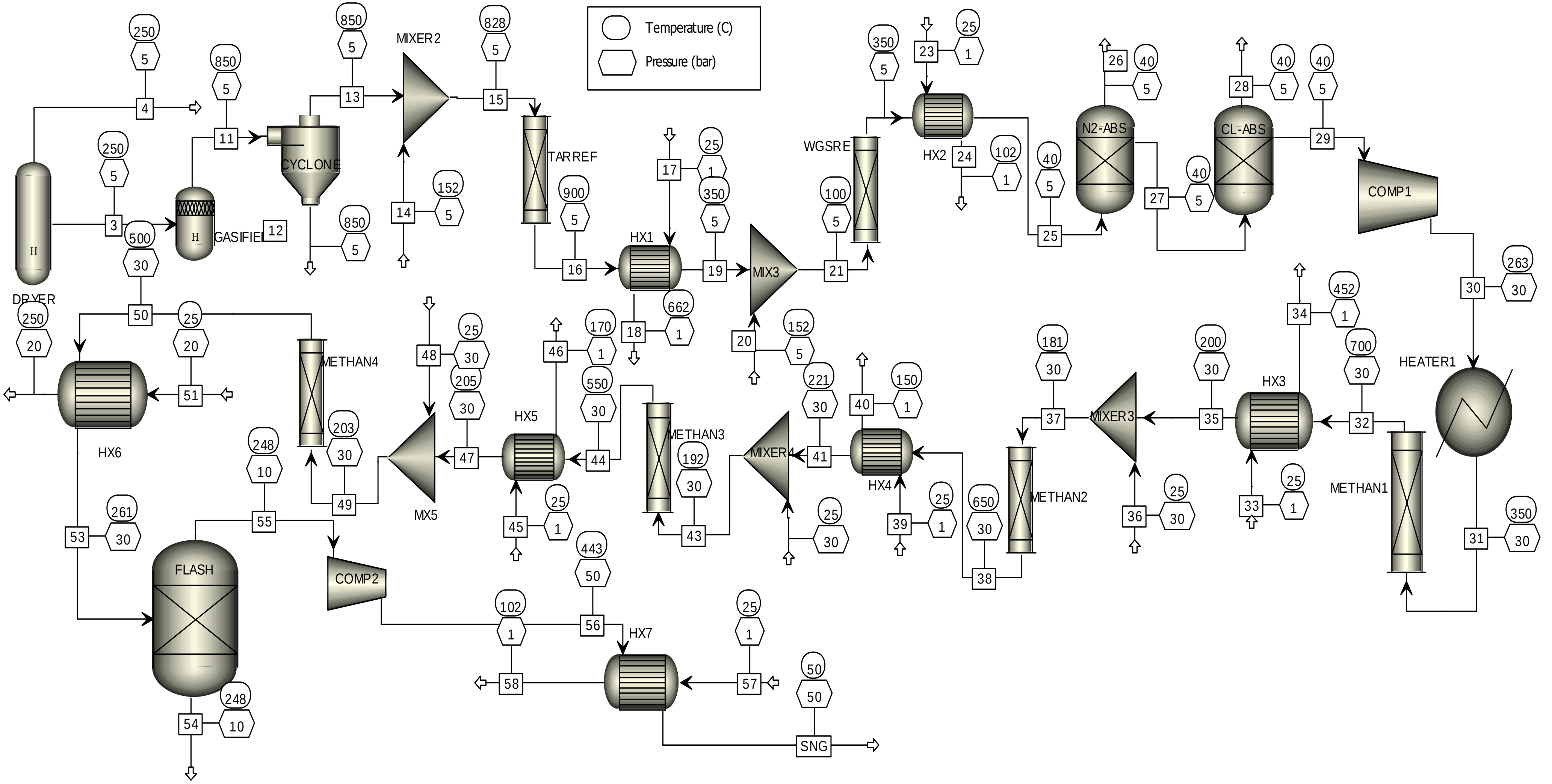

Figure 11.4:Flow sheet of Aspen Plus

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[52] Gasifier and Dryer are modelled as hierarchical modals

CHAPTER # 12

ENVIRONMENT IMPACT ASSESSMENT

12. Introduction:

The process of identifying the expected environmental consequences of a project and developing mitigation methods is known as environmental impact assessment (EIA). Before deciding, the primary purpose of EIA is to inform decision makers about the potential consequences of a project. EIA allows you to identify critical concerns and stakeholders early in the life of a plan, allowing you to resolve any negative consequences before final approval decisions are made. The EIA also includes a summary of the efforts taken to avoid, reduce, or eliminate these impacts.

12.1. Overview of EIA:

The US Environmental Protection Agency was the first to apply route analysis to predict the potential physical impact of environmental elements. Environmental science is the technology utilized to undertake such evaluations. The following are the major phenomena or pathways of influence:

- Noise and health consequences.
- The effects of water contamination.
- The effects of ecology, particularly the evaluation of endangered species.
- The effects of air pollution.
- Assessment of geological risks.
- Impacts of soil contamination.

12.2. Objectives of EIA:

- Ensure the environmental considerations are considered when making decisions.
- Ascertaining that all potential negative environmental consequences are detected and prevented or reduced.
- Getting the word out to the people about the plan.
- Enables individuals to investigate the underlying need for a project.
- Provides ample opportunity for people to spot problems.
- Assists a developer in creating a more publicly acceptable project.

12.3. Synthetic natural gas:

Synthetic natural gas (SNG) is an artificially created form of natural gas, which burns with a pale, faintly luminous flame, that can be made from coal, biomass, petroleum coke or solid waste. The carbon containing material may be gasified, and the resultant syngas can be transformed to methane, which is the primary component of natural gas. When compared to petroleum products, bio-SNG has a substantially lower carbon impact. SNG can be a low-carbon or even carbon-free alternative for fossil fuels, depending on the source fuel.

The environmental effect of SNG is determined by two major factors that can be made from coal, biomass, petroleum coke or solid waste. The carbon containing material may be gasified, and the resultant syngas can be transformed to methane, which is the primary component of natural gas. When compared to petroleum products, bio-SNG has a substantially lower carbon impact. SNG can be a low-carbon or even carbon-free alternative for fossil fuels, depending on the source fuel. The environmental effect of SNG is determined by two major factors:

1) The feedstock is used in the production of synthetic gas.
2) The fuel that petrol replaces in its final use.

12.3.1.Hazard identification:

Table 12.1: *Hazardous identification of SNG*

OSHA HCS 2012	• Flammable gas • Compressed gas • Simple Asphyxiant
Label elements	 
Hazard statements	• Extremely flammable gas • Contains gas under pressure, may explode when heated. • May displace oxygen, and cause rapid suffocation
Precautionary statements	• Avoid contact with heat, sparks, open flames, and/or hot surfaces. • Never extinguish unless the leak can be safely halted. • If possible, remove all ignition sources. • Keep out of direct sunlight. Keep in a well-ventilated area.

12.3.2.Composition/Information on ingredients:

Table 12.2: *Composition of SNG and their information*

Composition					
Chemical name	**Identifiers**	**%**	**LD50/LC50**	**Classification according to regulation**	**Comments**
Methane	CAS:74-82-8	94-98	NDA	OSHA HCS 2012: Flam. Gas 1; Press. Gas - Comp.; Simp. Asphyx.	NDA
Hydrogen	CAS:1333-74-0	3.1	NDA		NDA
Carbon dioxide	CAS:124-38-9	1.1	Inhalation-RateLC50-470000 ppm 30 Minute(s).		NDA

12.3.3.Health effects:

1) **Inhalation:**
   - **Acute**: This chemical is a fundamental asphyxiant. May displace or reduce the quantity of oxygen available for breathing, especially in congested areas. If this material is released in a small, poorly ventilated location (i.e. an enclosed or restricted space), an oxygen-deficient environment may result. Individuals exposed to such a setting may experience headaches, ringing in the ears, dizziness, tiredness, unconsciousness, nausea, vomiting, and sensory depression. Under some situations of overexposure, death may occur. Low oxygen levels are associated with increased respiration and pulse rate, emotional discomfort, atypical fatigue, nausea, vomiting, collapse, loss of consciousness, convulsive movements, respiratory collapse, and death
   - **Chronic:** No data available
2) **Skin:**
   - **Acute:** No adverse health consequences are anticipated under typical use circumstances.
   - **Chronic:** No data available
3) **Eye:**
   - **Acute:** No adverse health consequences are anticipated under typical use circumstances.
   - **Chronic:** No data available
4) **Ingestion:**
   - **Acute:** No adverse health consequences are anticipated under typical use circumstances
   - **Chronic:** No data available

12.3.4.First-aid measures:

1) **Inhalation:**

If the material is breathed, the victim should be moved to fresh air and placed in a comfortable breathing posture. If breathing is difficult, give oxygen. Artificial respiration should be used if the patient is not breathing. If the signs or symptoms persist, get medical treatment.

2) **Skin:**

If someone comes into contact with the chemical, properly wash their hands with soap and water. If you have skin irritation, get medical assistance. Before reuse infected clothes, wash it.

3) **Eye:**

If you have been exposed to SNG, clean your eyes for several minutes with caution. Remove any contact lenses that are present and readily removed. Repeat the rinse. Seek medical attention if the eye irritation persists.

4) **Ingestion:**

Ingestion is not predicted to be a usual form of chemical exposure.

5) **Indication of any immediate medical attention and special treatment needed:**

All treatments should be based on the patient's visible signs and feelings of pain. Ensure that medical personnel are informed of the material(s) involved and that proper precautions are taken. Rescuers should not attempt to collect chemically exposed people without adequate personal protection equipment. At the very least, a self-contained breathing apparatus (SCBA) is necessary. Victims who have any adverse effects as a consequence of overexposure to this gas mixture must seek medical attention. If necessary, rescuers should be sent to a hospital. Take a copy of the label and the MSDS to the victim(s)' doctor or other health care provider.

12.3.5.Fire-fighting measures:

- Flash point: -187.7 ^{o}C
- LEL: 5%

- UEL: 15%
- Autoignition temperature: 537.22 ⁰C

1) **Extinguishing media:**

Suitable extinguishing media	• Small fires: Dry chemicals or CO_2 • Large fires: Water spray or fog.
Unsuitable extinguishing media	No data available

2) **Special hazards arising from substance or mixture:**

Table 12.3: *Hazards arising from substance*

Unusual fire and explosion hazards	**Extremely flammable** • Will interact with air to generate explosive combinations. • Vapors might travel to the point of ignition and then flash back. • Fire-exposed cylinders may vent and emit flammable gas via pressure relief systems. • When heated, containers may explode. • Ruptured cylinders could possibly launch. • Produces a pale, slightly bright flame; air holding more than 14% methane burns quietly.
Hazardous combustion products	No data available

3) **Measures to be taken by fire fighters:**

- Protective apparel worn by structural firefighters provides very limited protection in fire circumstances; it is ineffective in spill scenarios where direct contact with the chemical is likely.
- Use a self-contained breathing device (SCBA) with positive pressure.
- Never put out a leaking gas fire unless the leak can be halted.
- Remove containers from the fire zone if possible.
- If a tank, rail car, or tank truck is on fire, ISOLATE for 1600 meters (1 mile) in all directions and contemplate an initial evacuation for 1600 meters (1 mile) in all directions.
- ALWAYS keep a safe distance from burning tanks.
- Fight fires from as far away as possible or utilize unmanned hose holders or monitor nozzles.
- Withdraw instantly if there is a rising sound from the venting safety mechanisms or if the tank is discolored.
- Flood containers with water until the fire has been extinguished.
- Avoid directing water at the source of the leak or safety devices; icing may develop.

- Use unsupervised hose holders or monitor nozzles for major flames; if this is not possible, leave the area and let the fire burn.

12.3.6.Accidental release measures:

Table 12.4: *Accidental release measurement*

Personal Precautions	• Unless wearing suitable protective clothes, do not handle broken containers or spilt material. • Do not walk through spilled material. Before entering, make sure the place is well ventilated.
Emergency procedures	• Remove ALL IGNITION SOURCES (no smoking, flares, sparks, or flames in the area). • As a first precaution, isolate the spill or leak spot for at least 100 metres (330 feet) in all directions. • If possible, stop the leak safely. Keep unauthorized people at bay. Avoid low-lying areas. Maintain your head upwind. • Consider first downwind evacuation for at least 800 metres (1/2 mile) for big spills. If an uncontrolled leak is discovered that cannot be halted by shutting off the nearest suitable valve or main supply valve (without danger), adopt an evacuation plan and contact the local fire department immediately.
Environmental precautions	• Prevent vapours from spreading through sewers, ventilation systems, and tight spaces.
Methods and material for containment	
Containment/Clean-up Measures	• Every equipment involved in the product's handling must be grounded. • Stop the leak if you can do so safely. If feasible, flip leaky containers so that gas rather than liquid escapes. • Spray water on the leak, spill area, or within the container to minimise vapours; do not pour water directly on the leak, spill area, or inside the container. • Do not aim water at the spill or the source of the leak. Isolate the area until the gas has dissipated.

12.3.7.Handling and storage:

1) **Handling:**
    - Keep out of heat and ignition sources.
    - Take precautions against static charges.
    - Ground any equipment used when handling the product.
    - Only use non-sparking tools. Only use with proper ventilation. Closed places should be ventilated before entering.
    - Be mindful of any indications of dizziness or exhaustion, especially if working in a poorly ventilated environment; lethal quantities of this gas combination may arise without any notable warning symptoms owing to olfactory fatigue or oxygen deprivation. Cylinders should be securely fastened to avoid dropping or being knocked over.
    - Cylinders should be securely fastened to avoid dropping or being knocked over.
2) **Storage:**
    - Store cylinders in dry, well-ventilated places away from sources of heat, ignition, and direct sunlight.
    - Do not allow the temperature in the storage area to reach 52 ºC (125 ºF). Cylinders must be stored away from the elements and preferably at a temperature of around 21 ºC (70 ºF).
    - Shield cylinders from physical damage. Cylinders should be securely fastened to avoid dropping or being knocked over.

12.3.8.Personal protection/exposure control:

Table 12.5: *Exposure limits and guidelines*

Exposure limits/ guidelines				
	Result	**Acgih**[53]	**Niosh**[54]	**Osha**[55]
Carbon dioxide	Twas[56]	5000 ppm twa	5000 ppm twa; 9000 mg/m^3 twa	5000 ppm twa; 9000 mg/m^3 twa
	Stels[57]	3000 ppm stel	30000 ppm stel; 54000 mg/m^3 stel	Not established
Methane	Twas	1000 ppm	Not established	Not established

1) **Engineering measures/control:**
    - There should be enough general ventilation. Ventilation rates should be proportional to the circumstances.
    - If necessary, use process enclosures, local exhaust ventilation, or other technological controls to keep airborne levels below recommended exposure limits.
    - Maintain appropriate airborne levels if exposure limits have not been determined. Explosion-proof electrical, ventilation, and/or lighting equipment should be used.

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[53] American Conference of Governmental Industrial Hygiene.

[54] National Institute of Occupational Safety and Health.

[55] Occupational Safety and Health Administration.

[56] Time-Weighted Averages are based on 8h/day, 40h/week exposures.

[57] Short Term Exposure Limits are based on 15-minute exposures.

2) **Personal protective equipment's (PPE's):**

- **Respiratory**: OSHA respirator requirements should be followed that can be found in 29 CFR 1910.134. If exposure limits are exceeded or symptoms occur, use an NIOSH/MSHA approved respirator.
- **Eye/Face**: Wear safety glasses.
- **Skin/Body**: Wear leather gloves when handling cylinders
- **Environmental exposure control:** Adhere to best practices for waste disposal and site management. Controls to prevent environmental release should be devised, including steps to avoid spills, air release, and river release.

Figure 12.1: *Personal prospective equipment (PPE)*

12.3.9.Stability and reactivity:

1) **Reactivity:**
   - Under typical conditions of usage, no adverse reactions have been seen.
2) **Chemical Stability:**
   - Stable
3) **Possibility of hazardous reactions:**
   - Hazardous polymerization will not occur.
4) **Conditions to avoid:**
   - Materials that are incompatible. Keep away from heat and ignition sources. Heat in excess.
5) **Incompatible materials:**
   - Intense reactions are caused by strong oxidizers (e.g., bromine pentafluoride, chlorine trifluoride, chlorine, fluorine, iodine heptafluoride, dioxygenyl tetrafluoroborate, dioxygen difluoride, trioxygen difluoride, liquid oxygen).
6) **Hazardous decomposition products:**
   - No data available.

12.3.10. Toxicological information:

Table 12.6: *Toxicological information of methane and carbon dioxide.*

Components		
Methane	74-82-8	• **Acute Toxicity:** Inhalation-Mouse LC50 • 326 g/m^3 2 Hour(s)
Carbon dioxide	124-38-9	• **Acute Toxicity:** Inhalation-Rat LC50 • 470000 ppm 30 Minute(s); Inhalation-Human TCLo • 7 pph; • **Behavioral:** Irritability; Brain and Coverings: Other degenerative changes; Nutritional and Gross Metabolic: Changes in Chemistry or Temperature: Body temperature decrease

12.3.11. Transport information:

Table 12.7: *Transport information of different international city*

	UN number	**UN proper shipping name**	**Transport hazard classes**	**Packing group**	**Environmental hazards**
Department of transportation	UN1954	Compressed gas, flammable, n.o.s. (Methane and Hydrogen)	2.1	NDA	NDA
TDG Australia	UN1954	Compressed gas, flammable, N.O.S. (Methane and Hydrogen)	2.1		Potentially marine pollutant
International air transport association	UN1954	Compressed gas, flammable, n.o.s. (Methane and Hydrogen)	2.1		NDA

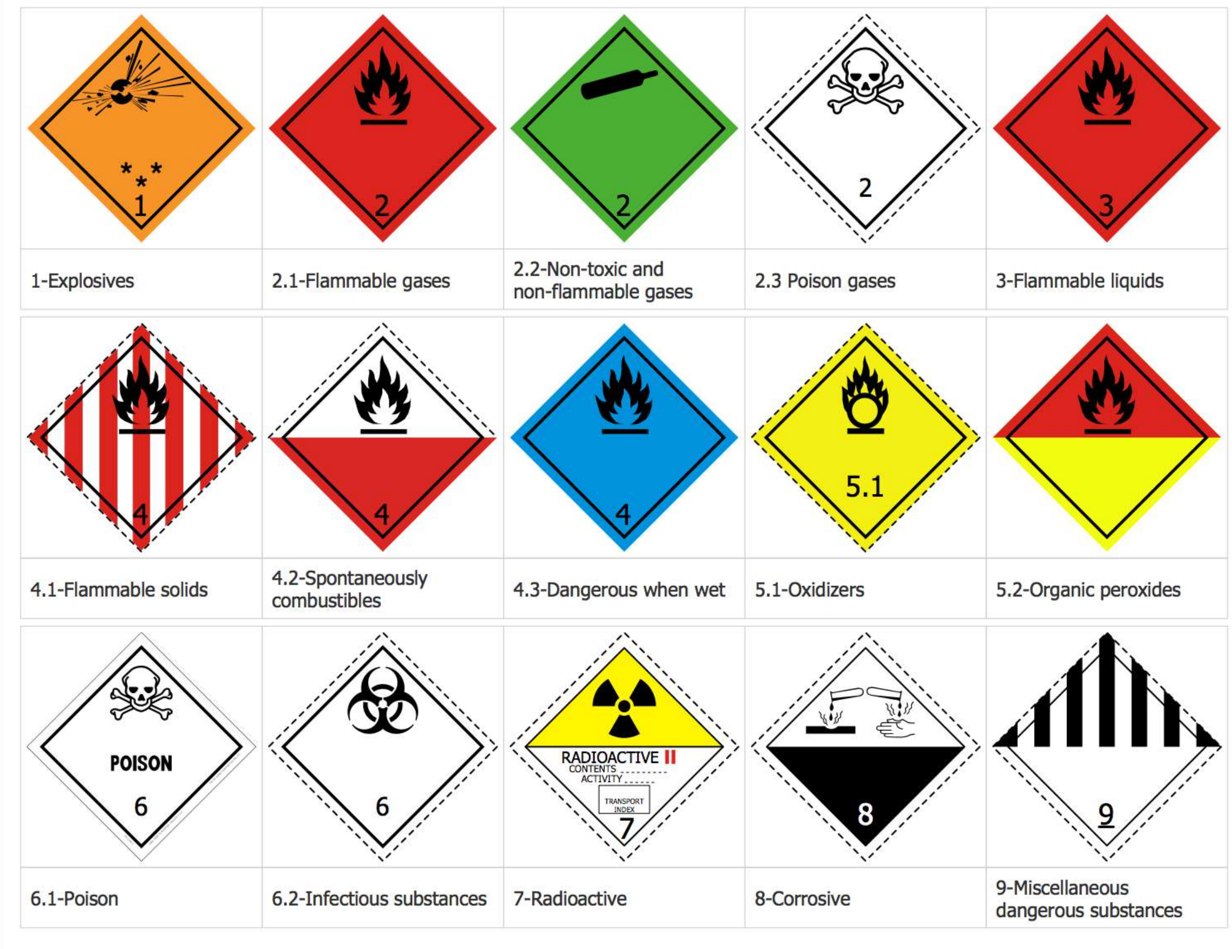

__Figure 12.2:__ Identification of different hazardous chemicals

- **Special precaution for user:**

Cylinders must be transported in a secure and adequately ventilated vehicle. The transportation of compressed gas cylinders in automobiles or closed-body vehicles might pose serious safety hazards. When transporting these cylinders in automobiles, ensure sure they are not exposed to extremely high temperatures (as might occur in an enclosed vehicle on a hot day). In addition, the automobile should be well-ventilated while in motion.

12.3.12. Environmental issues:

1) **Air emissions:**

When solid waste is gasified with oxygen and steam, two stream results.

- **Solid** ash is formed by decomposition of carbonaceous material via pyrolysis in the gasification chamber and can contribute as particulate pollutant.
- **Synthesis gas** containing range of hazardous components from carbon monoxide, hydrogen sulfide, nitrous oxide, and chlorine.
  1. The majority of emissions in formulating SNG results from gasification and gas cleaning section. Synthesis gas from gasification section contains excessive amounts of non-hydrocarbons and BTX that couldn’t only cause downstream pipeline and equipment damage but also can create an environmental hazard, when leaked.

2. Scrubbing of sour gases in gas cleaning section results in concentration buildup (unremoved loading) in solvent by which some working personnel might be exposed to. The absorbed gases are volatile and may leak into the environment due to pump seal inefficiencies.
3. The high temperature gradients along the methanation reactor results in creating a disturbance in convectional currents.
4. SNG consist primarily of methane, a greenhouse potent, and other non-hydrocarbon gases. Therefore, SNG must be enclosed in close cylinders and non-availability of ignition sources must be ensured.

2) Carbon monoxide:

Sources of carbon monoxide includes,

- Torr-gases
- Gasification
- Steam tar reformer
- Methanation

Carbon monoxide is primarily released in the form of volatiles from torrefaction of solid waste. These carbon oxides along with syngas is sent to tar reformer and water gas shift converter whereby carbon monoxide is converted to carbon dioxide and hydrogen.

3) Hydrogen sulfide:

Hydrogen sulfide is produced via reaction between elemental sulfur and hydrogen at elevated temperatures inside the gasifier. The effect of this reaction has farther effects, such as poisoning the catalyst, reducing the calorific value, contaminating the environment, then just corroding the material of construction.

4) Carbon dioxide:

Carbon dioxide results from devolatilization and reduction reactions in torrefaction and gasification reactor. The raw gas from gasifier is fed to water gas shift converter whereby carbon oxides are converted to carbon dioxides and hydrogen. Further in the downstream processing, CO_2 is removed via a side stream to maintain the proper methanation ratio.

5) Methane:

Methane is produced via hydrogenation of carbon oxides in the, presence of nickel-based catalyst, whose concentration in the SNG can vary from 94-98% depending on feed gas composition. Although methane is a widely known greenhouse gas that has emissions relatively lower than gas from fossil origin.

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APPENDICES

Appendix A

Design Considerations & Rating Data

Figures:

Tables:

1) Compressors:

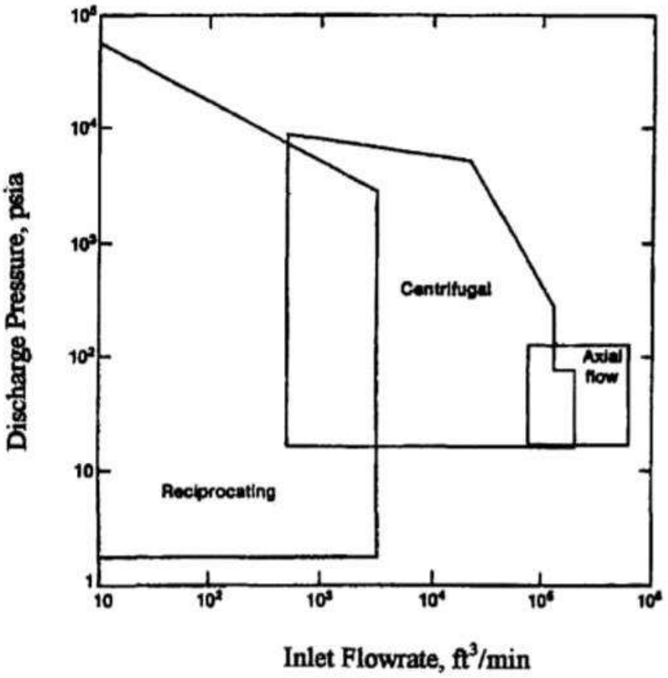


Figure A.1: *Compressor selection chart*

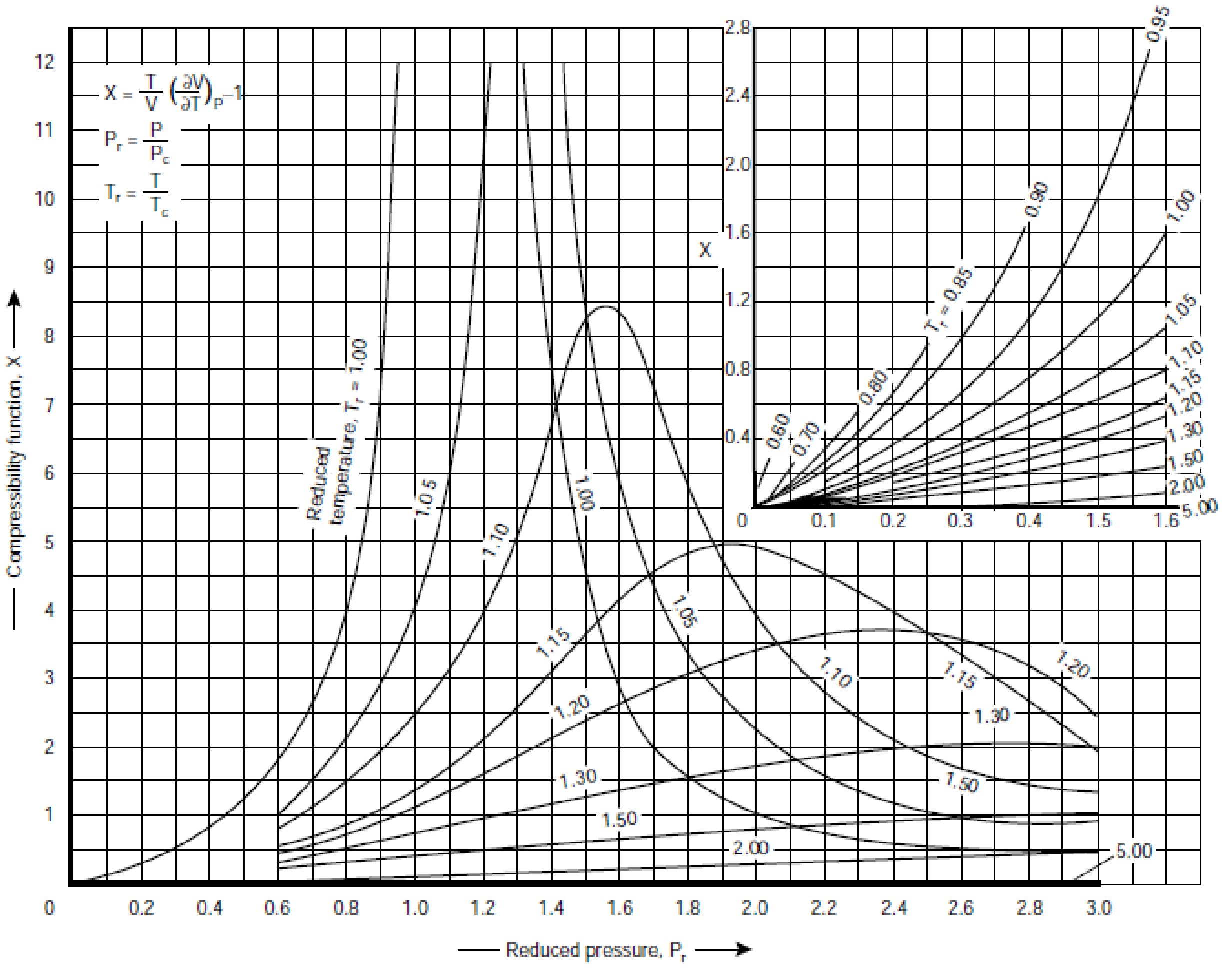


Figure A.2: *Compressibility function X chart*

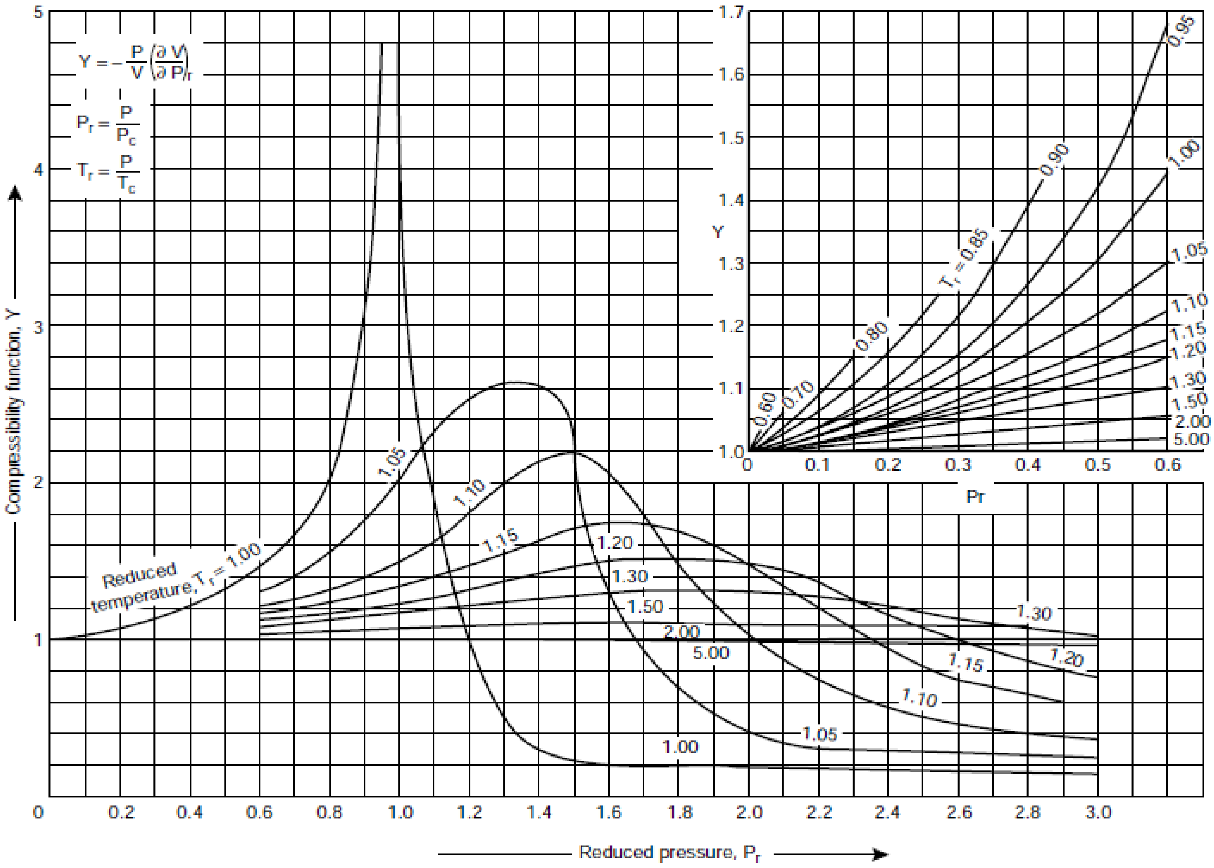


Figure A.3: *Compressibility function Y chart*

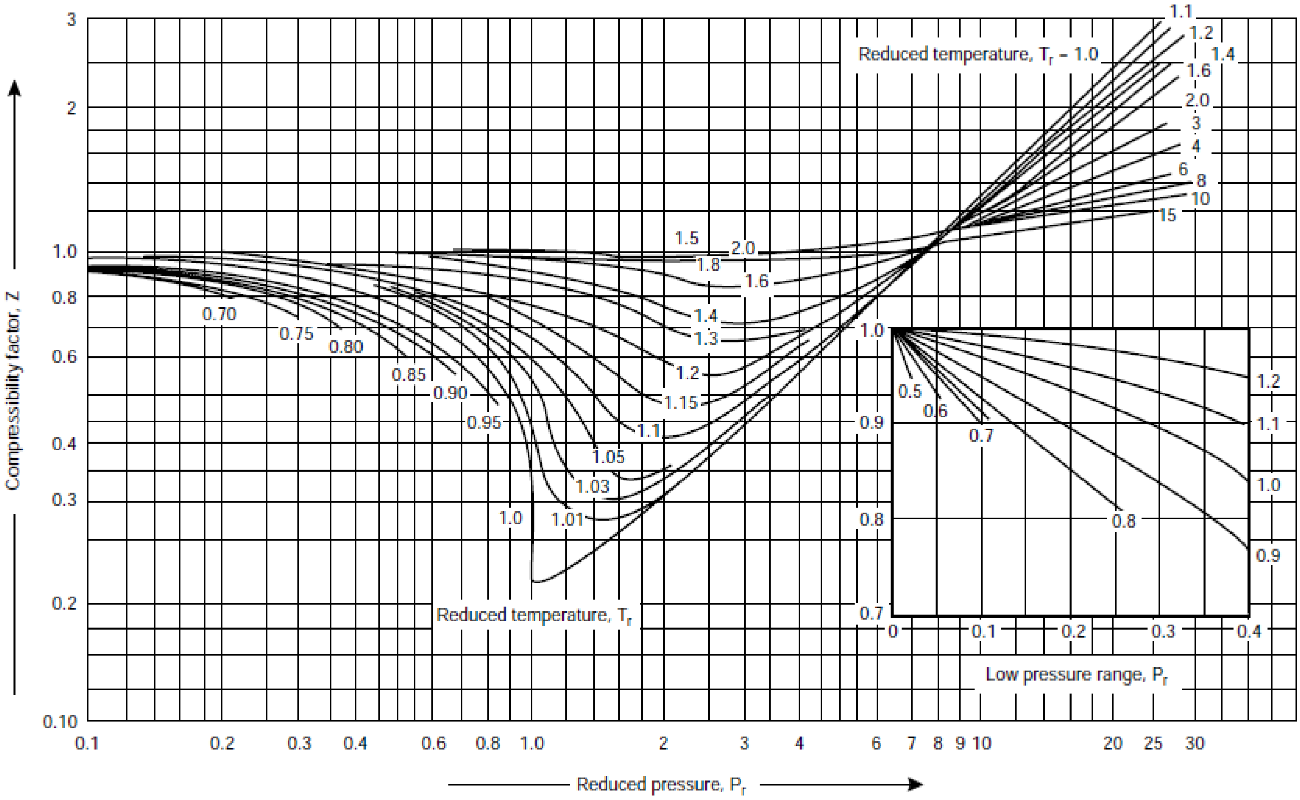


Figure A.4:*Super compressibility factor (Z) chart*

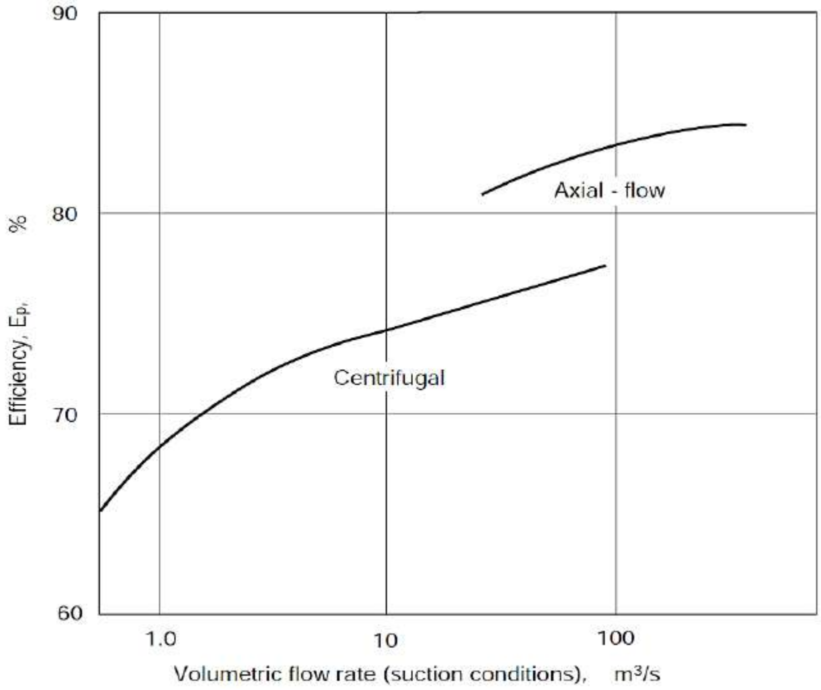
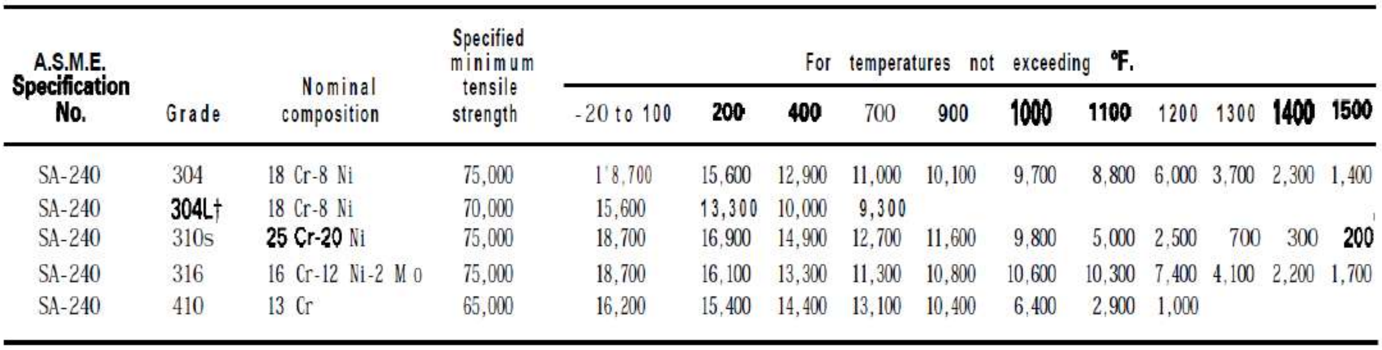


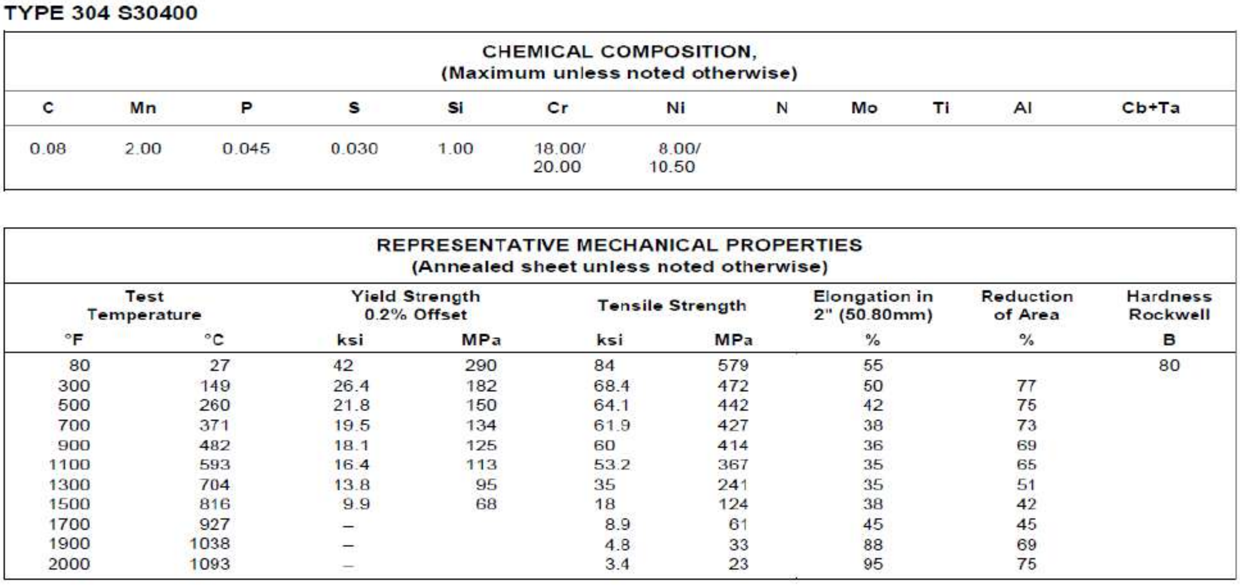
Figure A.5: *Compressor efficiency chart*

2) *Mechanical design Considerations:*

Table A.1: *Tensile strength of materials*



A.S.M.E. Specification No.	Grade	Nominal composition	Specified minimum tensile strength	For temperatures not exceeding °F.										
				-20 to 100	200	400	700	900	1000	1100	1200	1300	1400	1500
SA-240	304	18 Cr-8 Ni	75,000	1'8,700	15,600	12,900	11,000	10,100	9,700	8,800	6,000	3,700	2,300	1,400
SA-240	**304L†**	18 Cr-8 Ni	70,000	15,600	13,300	10,000	9,300							
SA-240	310s	**25 Cr-20** Ni	75,000	18,700	16,900	14,900	12,700	11,600	9,800	5,000	2,500	700	300	**200**
SA-240	316	16 Cr-12 Ni-2 Mo	75,000	18,700	16,100	13,300	11,300	10,800	10,600	10,300	7,400	4,100	2,200	1,700
SA-240	410	13 Cr	65,000	16,200	15,400	14,400	13,100	10,400	6,400	2,900	1,000			



TYPE 304 S30400

CHEMICAL COMPOSITION,
(Maximum unless noted otherwise)

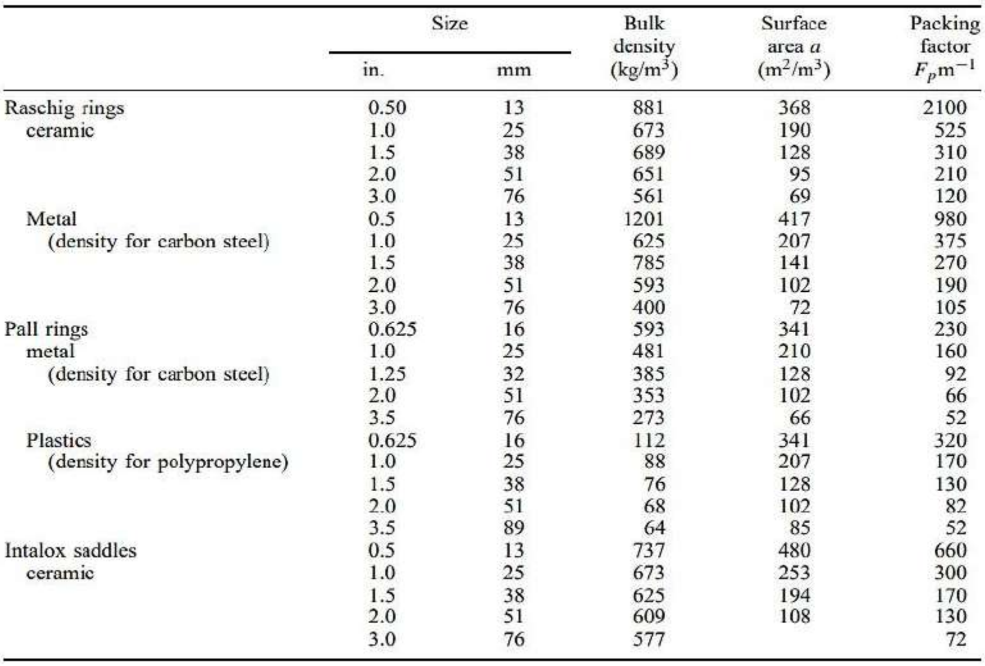
C	Mn	P	S	Si	Cr	Ni	N	Mo	Ti	Al	Cb+Ta
0.08	2.00	0.045	0.030	1.00	18.00/ 20.00	8.00/ 10.50					

REPRESENTATIVE MECHANICAL PROPERTIES
(Annealed sheet unless noted otherwise)

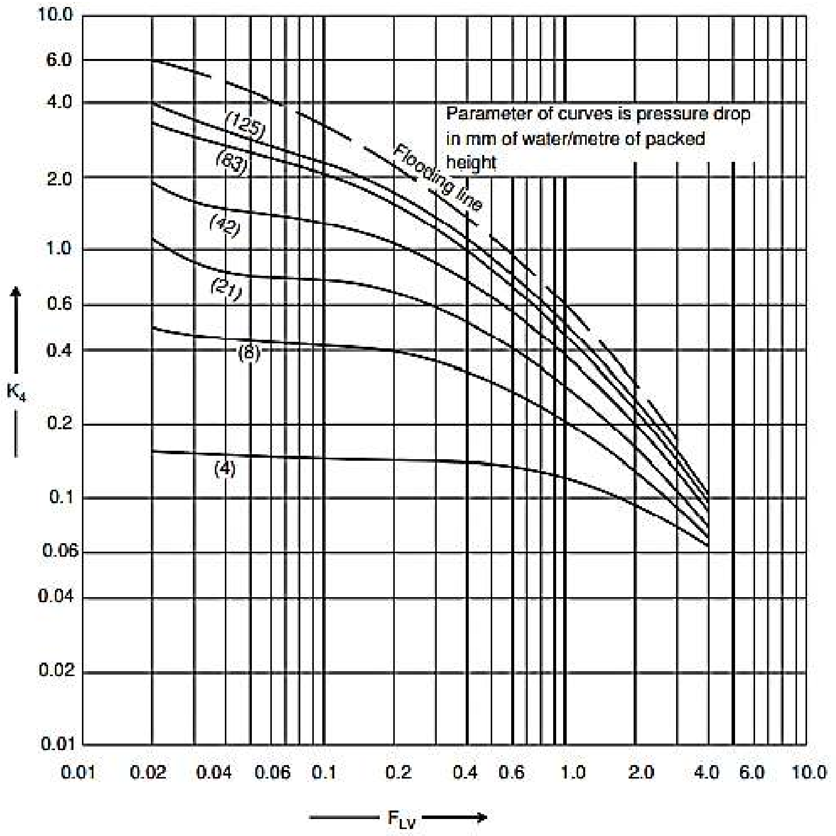
Test Temperature		Yield Strength 0.2% Offset		Tensile Strength		Elongation in 2" (50.80mm)	Reduction of Area	Hardness Rockwell
°F	°C	ksi	MPa	ksi	MPa	%	%	B
80	27	42	290	84	579	55		80
300	149	26.4	182	68.4	472	50	77	
500	260	21.8	150	64.1	442	42	75	
700	371	19.5	134	61.9	427	38	73	
900	482	18.1	125	60	414	36	69	
1100	593	16.4	113	53.2	367	35	65	
1300	704	13.8	95	35	241	35	51	
1500	816	9.9	68	18	124	38	42	
1700	927	–		8.9	61	45	45	
1900	1038	–		4.8	33	88	69	
2000	1093	–		3.4	23	95	75	

3) Absorption Design Consideration:

Table A.2: *Design data for various packing*



	Size		Bulk density (kg/m^3)	Surface area a (m^2/m^3)	Packing factor F_pm^{-1}
	in.	mm			
Raschig rings ceramic	0.50	13	881	368	2100
	1.0	25	673	190	525
	1.5	38	689	128	310
	2.0	51	651	95	210
	3.0	76	561	69	120
Metal (density for carbon steel)	0.5	13	1201	417	980
	1.0	25	625	207	375
	1.5	38	785	141	270
	2.0	51	593	102	190
	3.0	76	400	72	105
Pall rings metal (density for carbon steel)	0.625	16	593	341	230
	1.0	25	481	210	160
	1.25	32	385	128	92
	2.0	51	353	102	66
	3.5	76	273	66	52
Plastics (density for polypropylene)	0.625	16	112	341	320
	1.0	25	88	207	170
	1.5	38	76	128	130
	2.0	51	68	102	82
	3.5	89	64	85	52
Intalox saddles ceramic	0.5	13	737	480	660
	1.0	25	673	253	300
	1.5	38	625	194	170
	2.0	51	609	108	130
	3.0	76	577		72



$$F_{LV} = \frac{L_W^*}{V_W^*}\sqrt{\frac{\rho_V}{\rho_L}}$$

Generalised pressure drop correlation, adapted from a figure by the Norton Co. with permission

Figure A.6: *Generalized pressure drop correlation,*

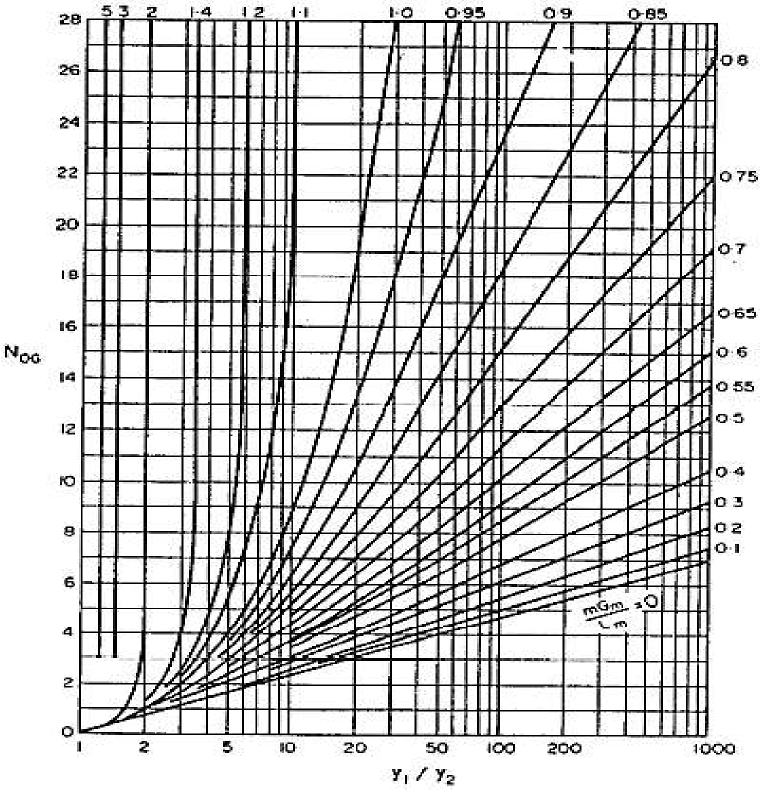


Figure 11.40. Number of transfer units N_{OG} as a function of y_1/y_2 with mG_m/L_m as parameter

Figure A.7: *Number of transfer units N_{OG} as a function of y1/y2 with mGm/Lm as parameter*

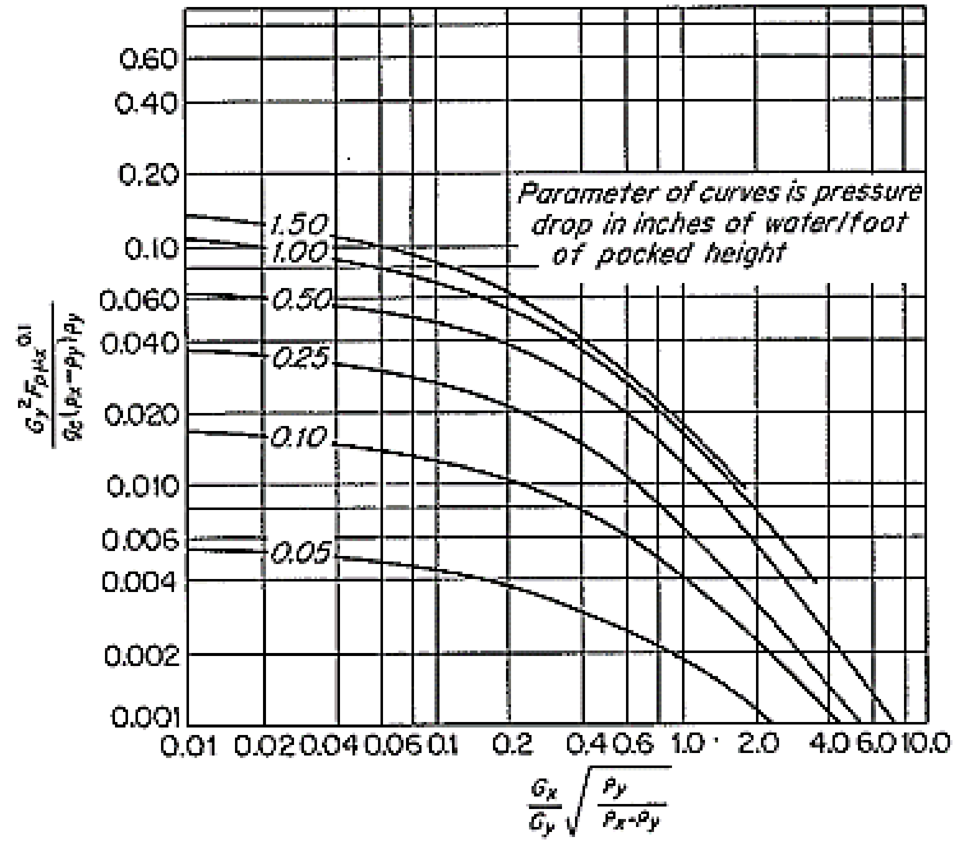


Figure A.8: *Generalized correlation for pressure drop in packed column*

Appendix B

Cost Estimation

Figures:

Tables:

APPENDIX-B

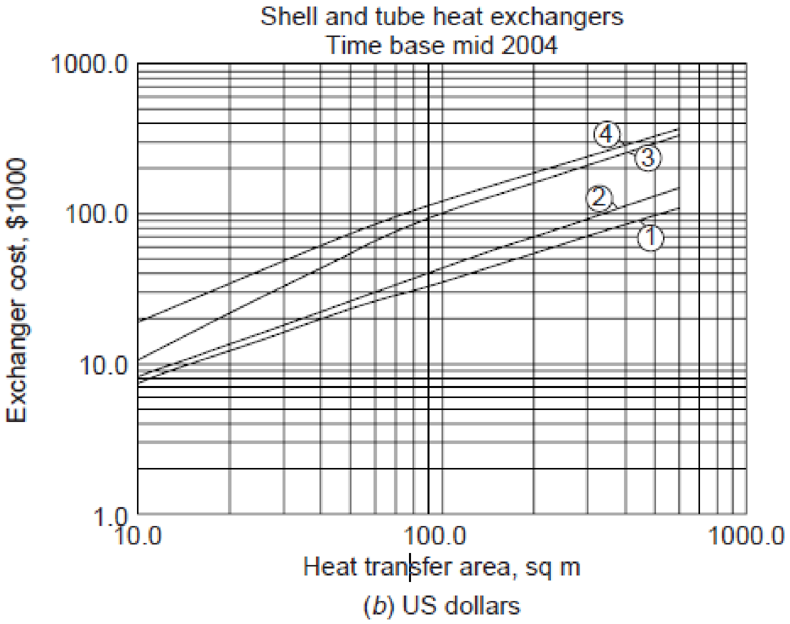
1) Chemical Engineering Plant Cost Index:

Table B.1: *Chemical engineering plant cost index*

CEPCI 2001 to Present

Year	CEPCI
2022 Dec Prlm	808.7
2022 Nov	814.6
2022 Oct	816.2
2022 Sep	821.3
2022 Aug	824.5
2022 Jul	829.8
2022 Jun	832.6
2022 May	831.1
2022 Apr	816.3
2022 Mar	803.6
2022 Feb	801.3
2022 Jan	797.6
2021 Dec	776.3
2021 Nov	773.1
2021 Oct	761.4

2) Cost of multi-tubular reactors



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

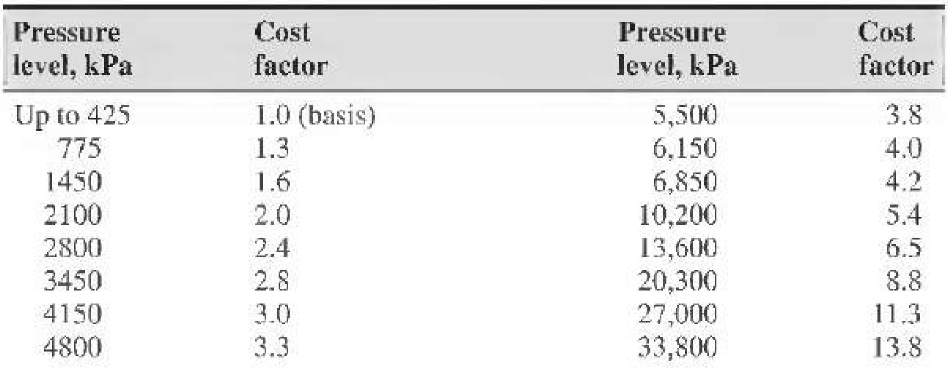
Pressure factors	
1–10 bar	× 1.0
10–20	× 1.1
20–30	× 1.25
30–50	× 1.3
50–70	× 1.5

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

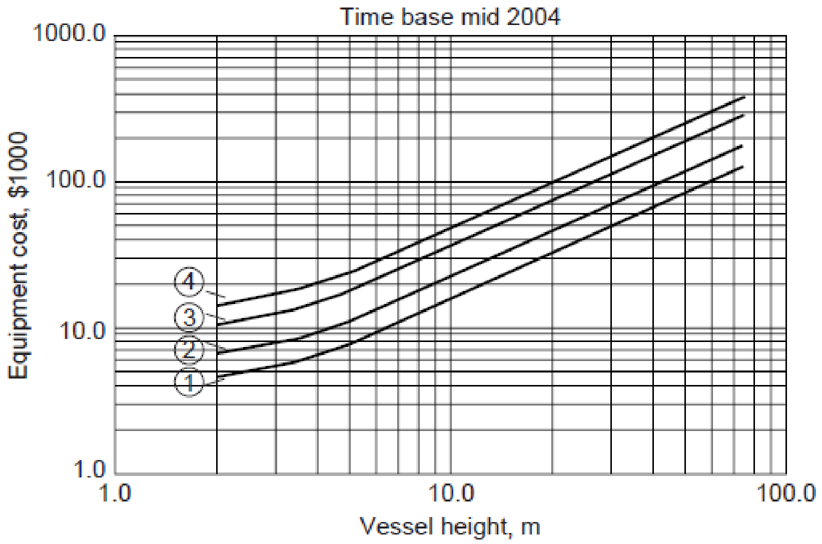
Figure B.1: *Cost of multi-tubular reactors*

3) Cost of Pressure Vessel:

Table B.2: *Cost factors to account for internal pressure levels of vessels*



Pressure level, kPa	Cost factor	Pressure level, kPa	Cost factor
Up to 425	1.0 (basis)	5,500	3.8
775	1.3	6,150	4.0
1450	1.6	6,850	4.2
2100	2.0	10,200	5.4
2800	2.4	13,600	6.5
3450	2.8	20,300	8.8
4150	3.0	27,000	11.3
4800	3.3	33,800	13.8



(*b*) US dollars

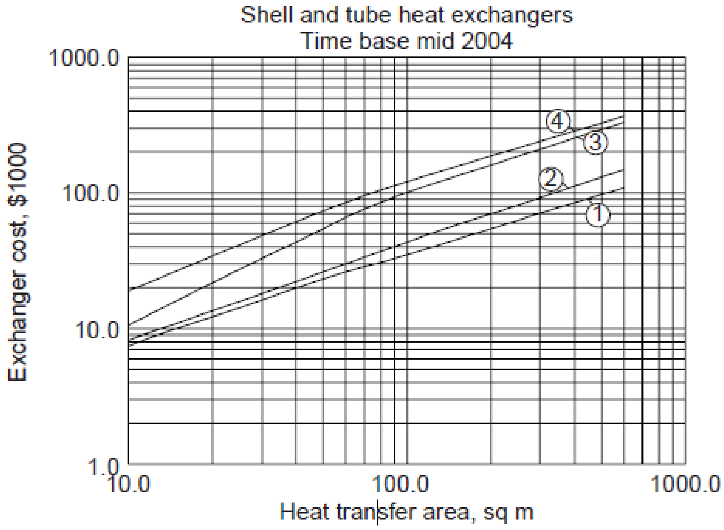
Diameter, m

①—0.5 ③—2.0
②—1.0 ④—3.0

Material factors	
C.S.	× 1.0
S.S.	× 2.0
Monel	× 3.4
S.S. clad	× 1.5
Monel clad	× 2.1

Pressure factors	
1–5 bar	× 1.0
5–10	× 1.1
10–20	× 1.2
20–30	× 1.4
30–40	× 1.6
40–50	× 1.8
50–60	× 2.2

Temperature up to 300°C



(*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.

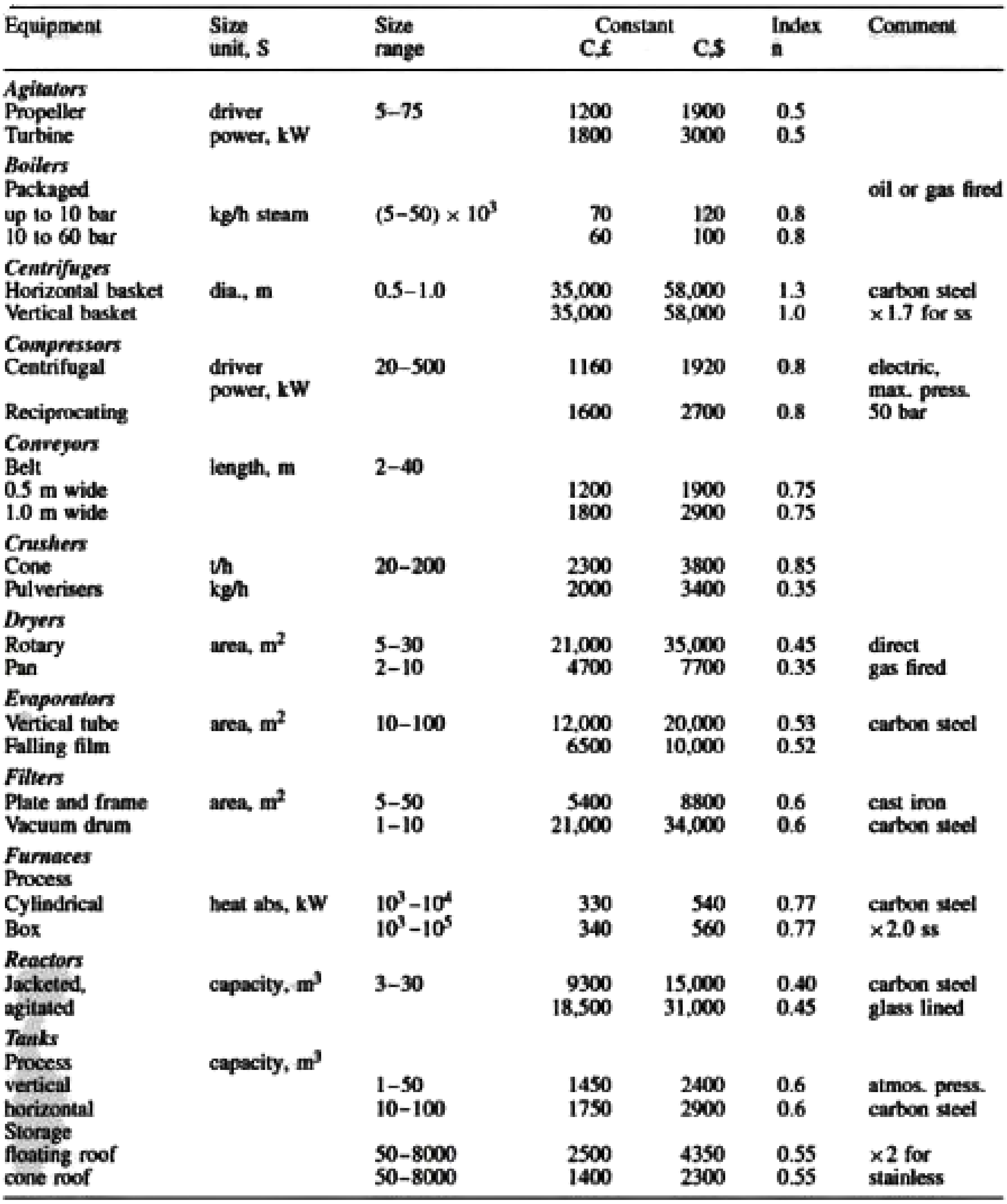
Pressure factors	
1–10 bar	× 1.0
10–20	× 1.1
20–30	× 1.25
30–50	× 1.3
50–70	× 1.5

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

Figure B.2: *Cost of WHB and shell & tube heat exchangers:*

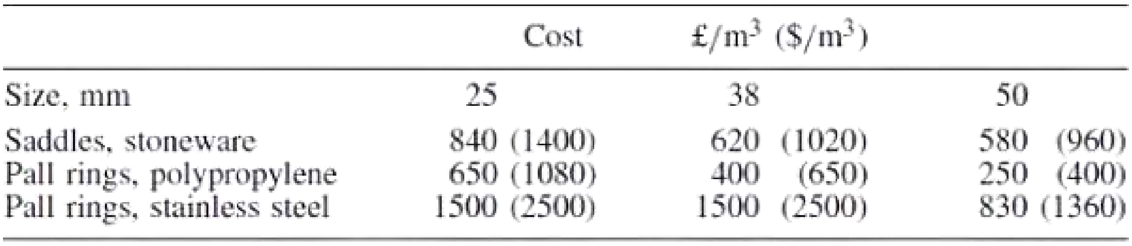
4) Cost of equipment:

Table B.3: *Cost of equipment*



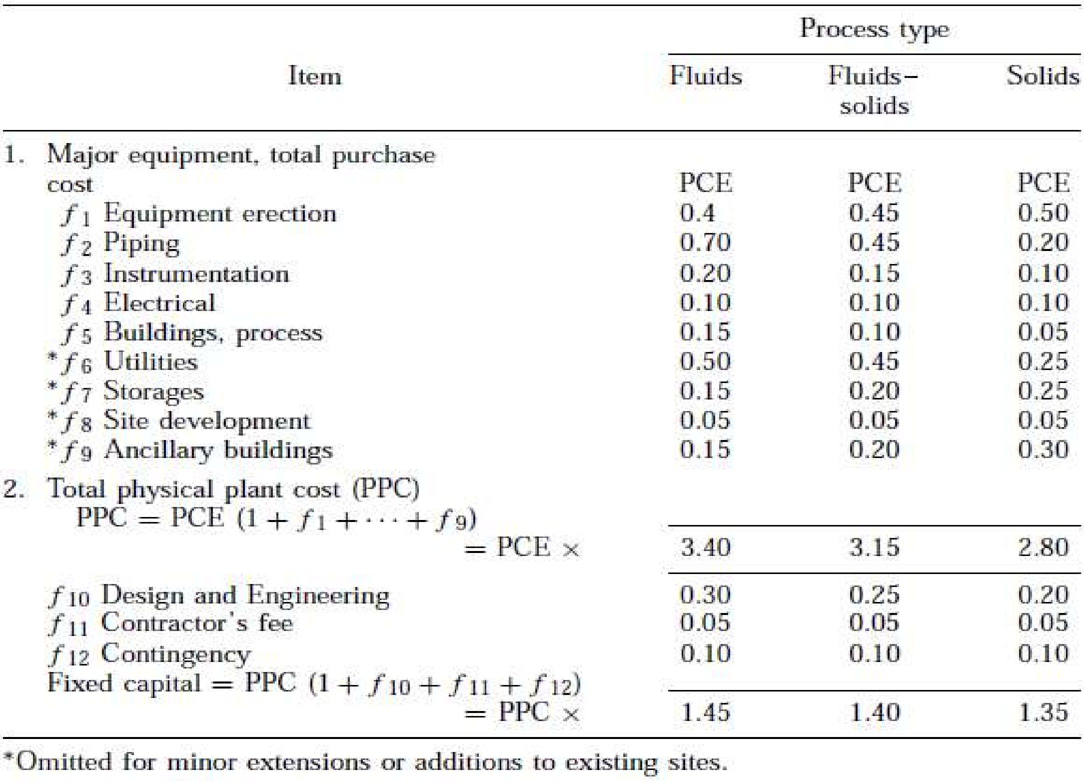
Equipment	Size unit, S	Size range	Constant		Index n	Comment
			C£	C$		
Agitators						
Propeller	driver power, kW	5–75	1200	1900	0.5	
Turbine			1800	3000	0.5	
Boilers						
Packaged						oil or gas fired
up to 10 bar	kg/h steam	(5–50) × 10^3	70	120	0.8	
10 to 60 bar			60	100	0.8	
Centrifuges						
Horizontal basket	dia., m	0.5–1.0	35,000	58,000	1.3	carbon steel
Vertical basket			35,000	58,000	1.0	×1.7 for ss
Compressors						
Centrifugal	driver power, kW	20–500	1160	1920	0.8	electric, max. press.
Reciprocating			1600	2700	0.8	50 bar
Conveyors						
Belt	length, m	2–40				
0.5 m wide			1200	1900	0.75	
1.0 m wide			1800	2900	0.75	
Crushers						
Cone	t/h	20–200	2300	3800	0.85	
Pulverisers	kg/h		2000	3400	0.35	
Dryers						
Rotary	area, m^2	5–30	21,000	35,000	0.45	direct
Pan		2–10	4700	7700	0.35	gas fired
Evaporators						
Vertical tube	area, m^2	10–100	12,000	20,000	0.53	carbon steel
Falling film			6500	10,000	0.52	
Filters						
Plate and frame	area, m^2	5–50	5400	8800	0.6	cast iron
Vacuum drum		1–10	21,000	34,000	0.6	carbon steel
Furnaces						
Process						
Cylindrical	heat abs, kW	10^3–10^4	330	540	0.77	carbon steel
Box		10^3–10^5	340	560	0.77	×2.0 ss
Reactors						
Jacketed,	capacity, m^3	3–30	9300	15,000	0.40	carbon steel
agitated			18,500	31,000	0.45	glass lined
Tanks						
Process	capacity, m^3					
vertical		1–50	1450	2400	0.6	atmos. press.
horizontal		10–100	1750	2900	0.6	carbon steel
Storage						
floating roof		50–8000	2500	4350	0.55	×2 for
cone roof		50–8000	1400	2300	0.55	stainless

Table B.4: *Cost of column packing*



	Cost	$\pounds/m^3$ ($\$/m^3$)	
Size, mm	25	38	50
Saddles, stoneware	840 (1400)	620 (1020)	580 (960)
Pall rings, polypropylene	650 (1080)	400 (650)	250 (400)
Pall rings, stainless steel	1500 (2500)	1500 (2500)	830 (1360)

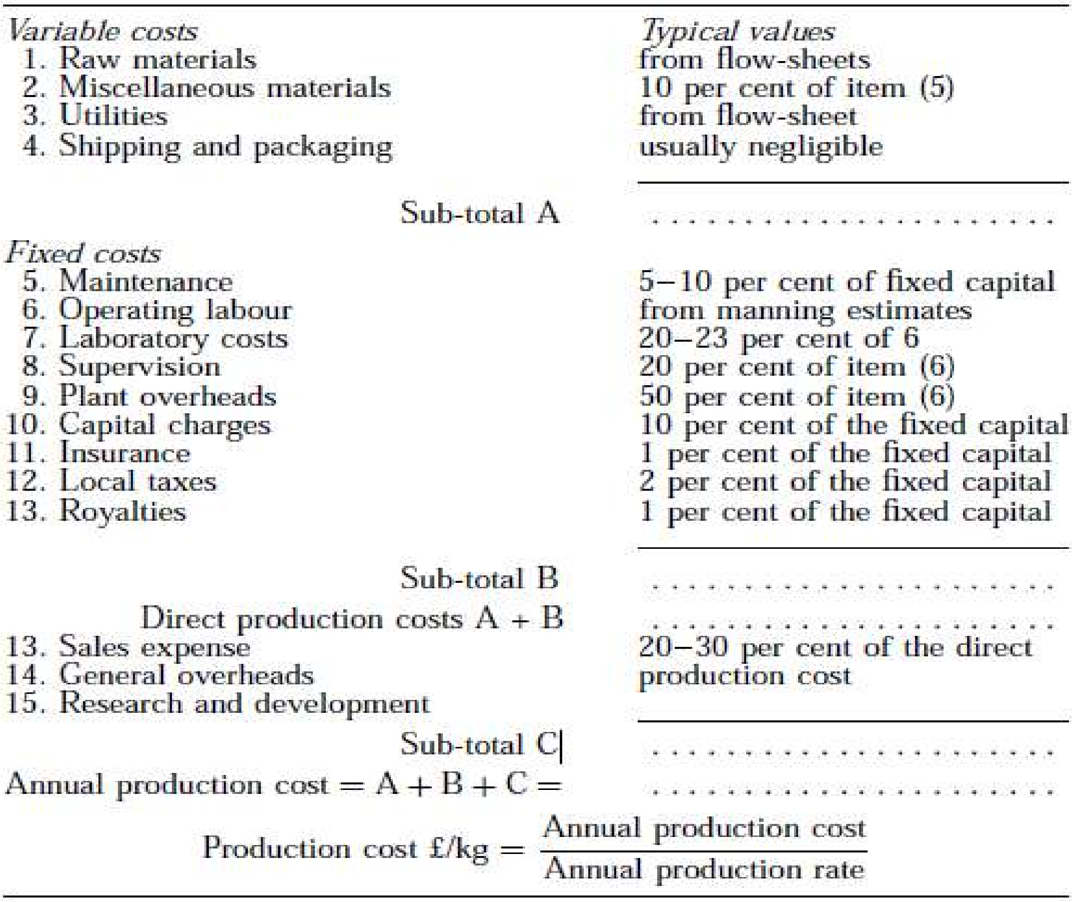
Table B.5: *Factors for cost estimation*



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
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.

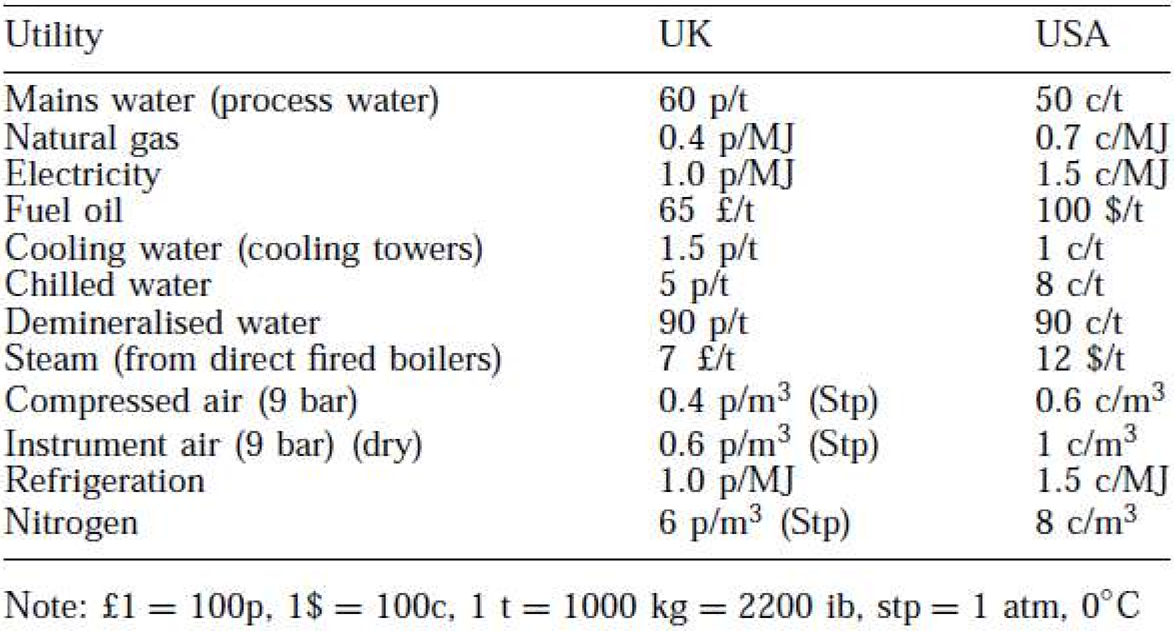
Table B.6: *Total production cost*



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 B.7: *Cost of utilities.*

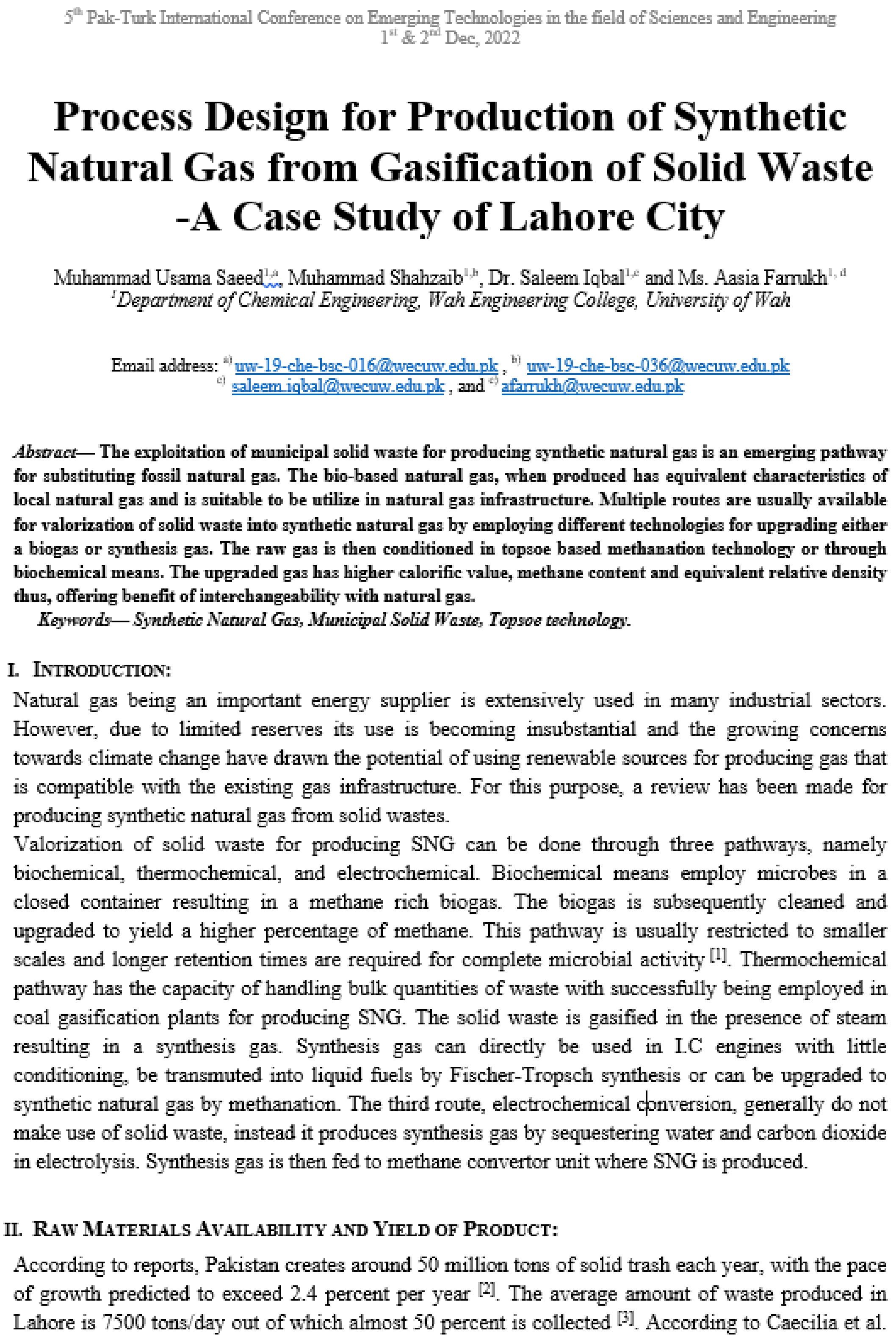


Utility	UK	USA
Mains water (process water)	60 p/t	50 c/t
Natural gas	0.4 p/MJ	0.7 c/MJ
Electricity	1.0 p/MJ	1.5 c/MJ
Fuel oil	65 £/t	100 $/t
Cooling water (cooling towers)	1.5 p/t	1 c/t
Chilled water	5 p/t	8 c/t
Demineralised water	90 p/t	90 c/t
Steam (from direct fired boilers)	7 £/t	12 $/t
Compressed air (9 bar)	0.4 p/m^3 (Stp)	0.6 c/m^3
Instrument air (9 bar) (dry)	0.6 p/m^3 (Stp)	1 c/m^3
Refrigeration	1.0 p/MJ	1.5 c/MJ
Nitrogen	6 p/m^3 (Stp)	8 c/m^3

Note: £1 = 100p, 1$ = 100c, 1 t = 1000 kg = 2200 ib, stp = 1 atm, 0°C

ACHIEVEMENT

ACHIEVEMENT



5th Pak-Turk International Conference on Emerging Technologies in the field of Sciences and Engineering
1st & 2nd Dec, 2022

Process Design for Production of Synthetic Natural Gas from Gasification of Solid Waste -A Case Study of Lahore City

Muhammad Usama Saeed[1,a], Muhammad Shahzaib[1,b], Dr. Saleem Iqbal[1,c] and Ms. Aasia Farrukh[1, d]
[1]*Department of Chemical Engineering, Wah Engineering College, University of Wah*

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[c)] saleem.iqbal@wecuw.edu.pk , and [c)] afarrukh@wecuw.edu.pk

Abstract— **The exploitation of municipal solid waste for producing synthetic natural gas is an emerging pathway for substituting fossil natural gas. The bio-based natural gas, when produced has equivalent characteristics of local natural gas and is suitable to be utilize in natural gas infrastructure. Multiple routes are usually available for valorization of solid waste into synthetic natural gas by employing different technologies for upgrading either a biogas or synthesis gas. The raw gas is then conditioned in topsoe based methanation technology or through biochemical means. The upgraded gas has higher calorific value, methane content and equivalent relative density thus, offering benefit of interchangeability with natural gas.**

Keywords— Synthetic Natural Gas, Municipal Solid Waste, Topsoe technology.

I. INTRODUCTION:

Natural gas being an important energy supplier is extensively used in many industrial sectors. However, due to limited reserves its use is becoming insubstantial and the growing concerns towards climate change have drawn the potential of using renewable sources for producing gas that is compatible with the existing gas infrastructure. For this purpose, a review has been made for producing synthetic natural gas from solid wastes.

Valorization of solid waste for producing SNG can be done through three pathways, namely biochemical, thermochemical, and electrochemical. Biochemical means employ microbes in a closed container resulting in a methane rich biogas. The biogas is subsequently cleaned and upgraded to yield a higher percentage of methane. This pathway is usually restricted to smaller scales and longer retention times are required for complete microbial activity [1]. Thermochemical pathway has the capacity of handling bulk quantities of waste with successfully being employed in coal gasification plants for producing SNG. The solid waste is gasified in the presence of steam resulting in a synthesis gas. Synthesis gas can directly be used in I.C engines with little conditioning, be transmuted into liquid fuels by Fischer-Tropsch synthesis or can be upgraded to synthetic natural gas by methanation. The third route, electrochemical conversion, generally do not make use of solid waste, instead it produces synthesis gas by sequestering water and carbon dioxide in electrolysis. Synthesis gas is then fed to methane convertor unit where SNG is produced.

II. RAW MATERIALS AVAILABILITY AND YIELD OF PRODUCT:

According to reports, Pakistan creates around 50 million tons of solid trash each year, with the pace of growth predicted to exceed 2.4 percent per year [2]. The average amount of waste produced in Lahore is 7500 tons/day out of which almost 50 percent is collected [3]. According to Caecilia et al.

ACHIEVEMENT

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for attending as an **Oral Presenter** at the **5th International Pak-Turk Conference on Emerging Technologies in the field of Sciences & Engineering (ETSE-2022)** organized by the **University of Wah** on **1st & 2nd December 2022**

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Production of Synthetic Natural Gas (SNG) through gasification of biomass (food Waste).

(Chemical Department, University of Wah, Wah)

of your university has been approved for financial assistance by PEC

CONGRATULATIONS

It is required to complete this Design Project in accordance with the PEC standards so it can be included in the Capstone Expo-2023 and have it uploaded to the PEC E-library.

ENGR. MIR MASOOD RASHID Convener, PPDC, PEC	ENGR. DR. NASIR M. KHAN Registrar, PEC

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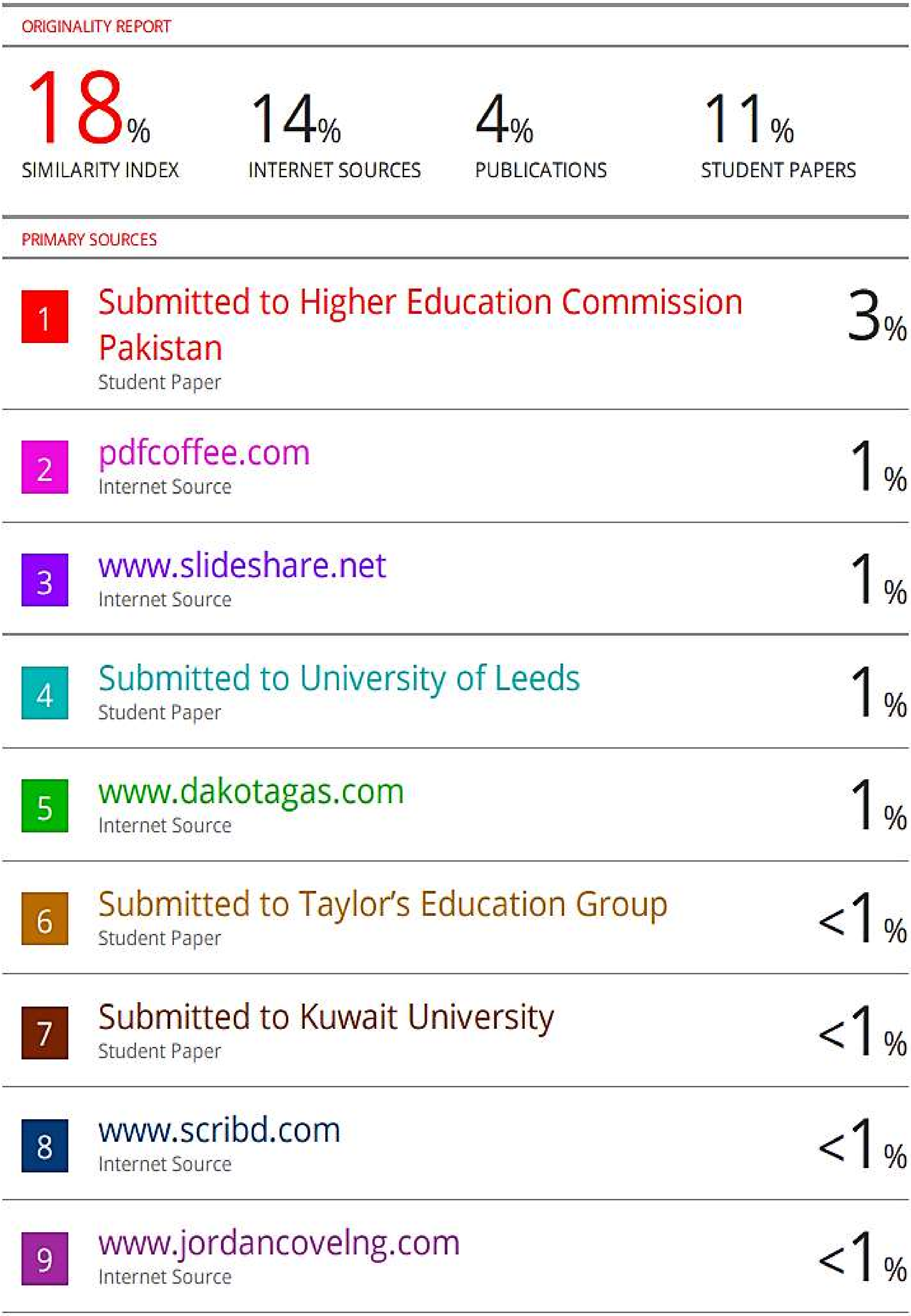

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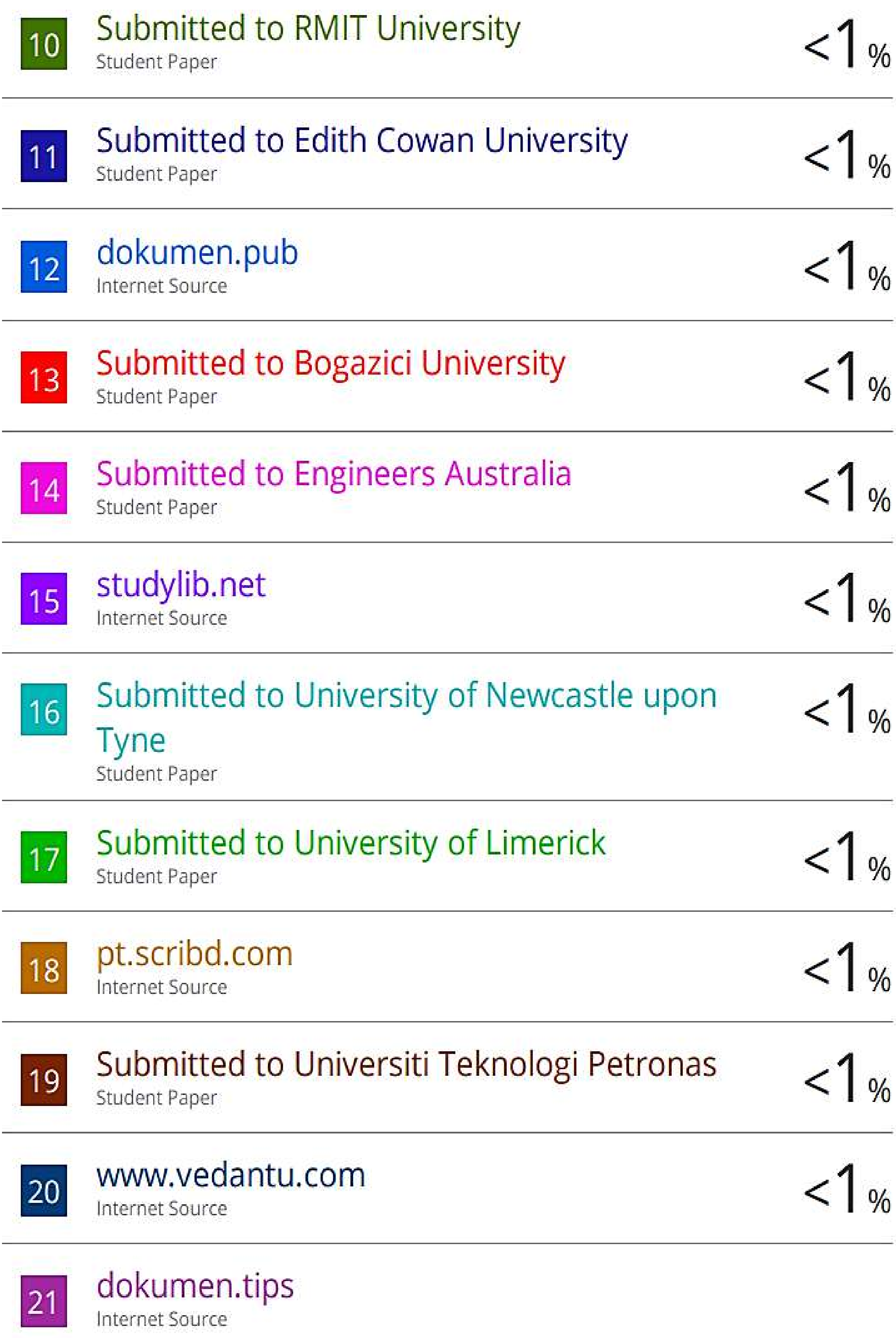

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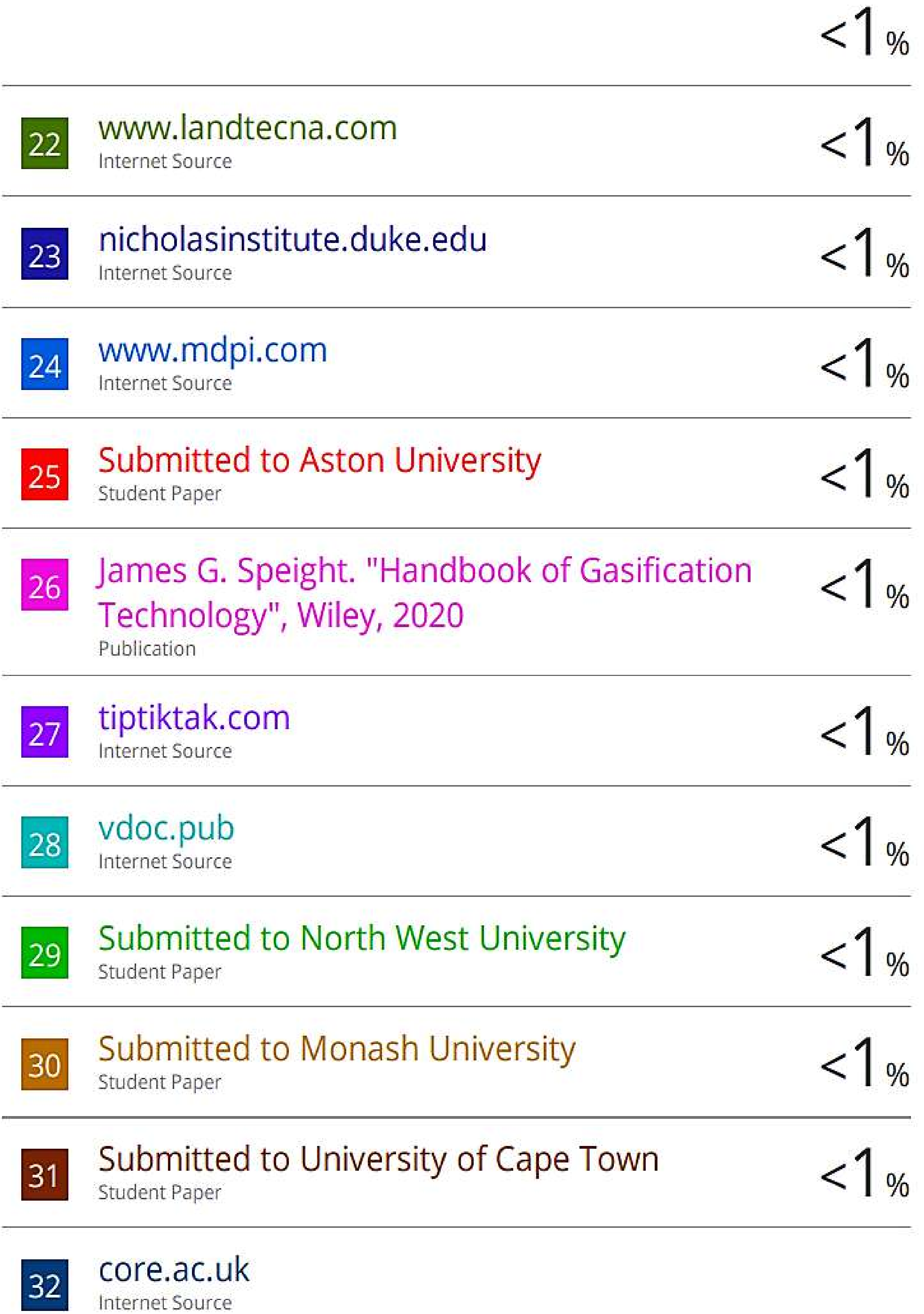

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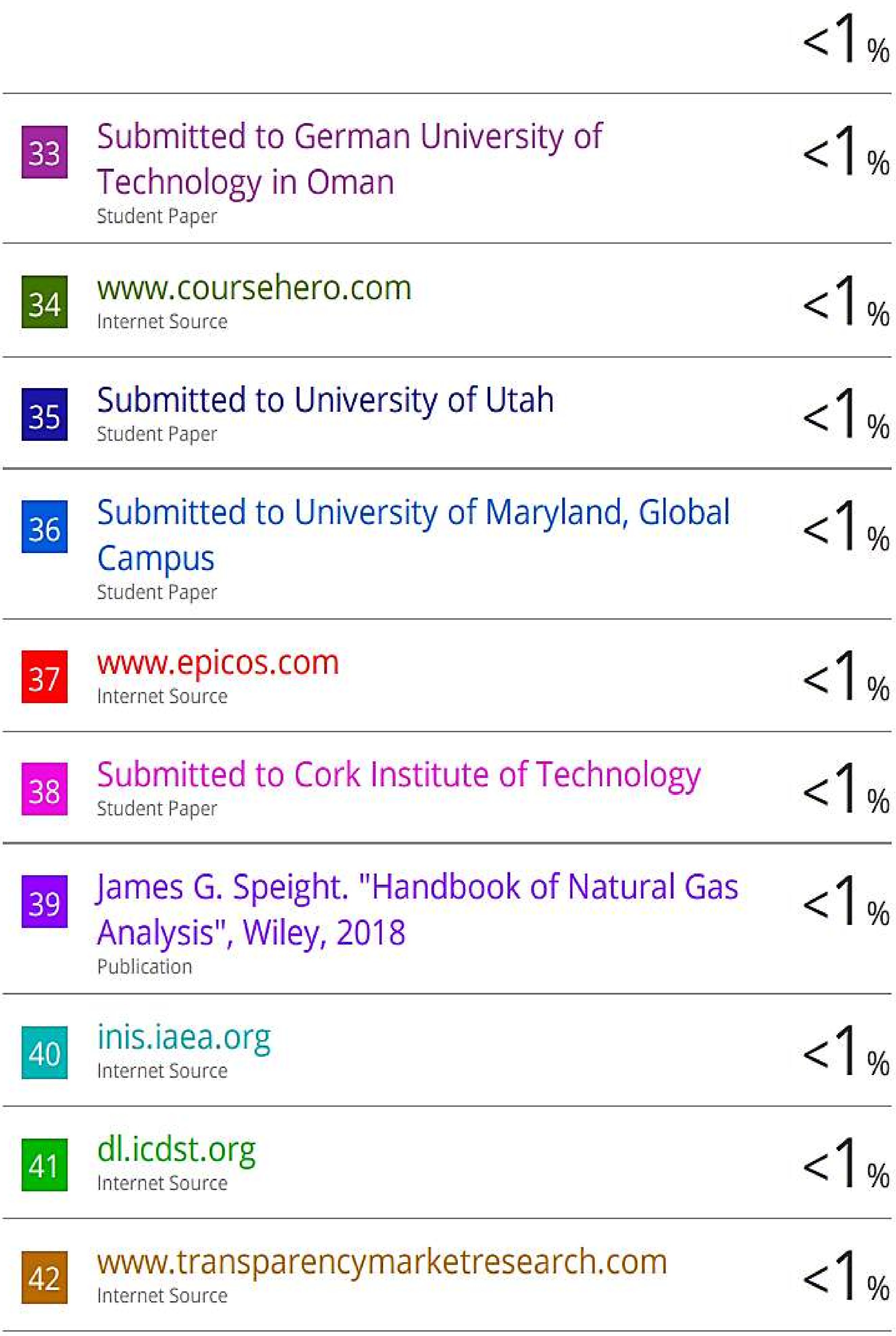

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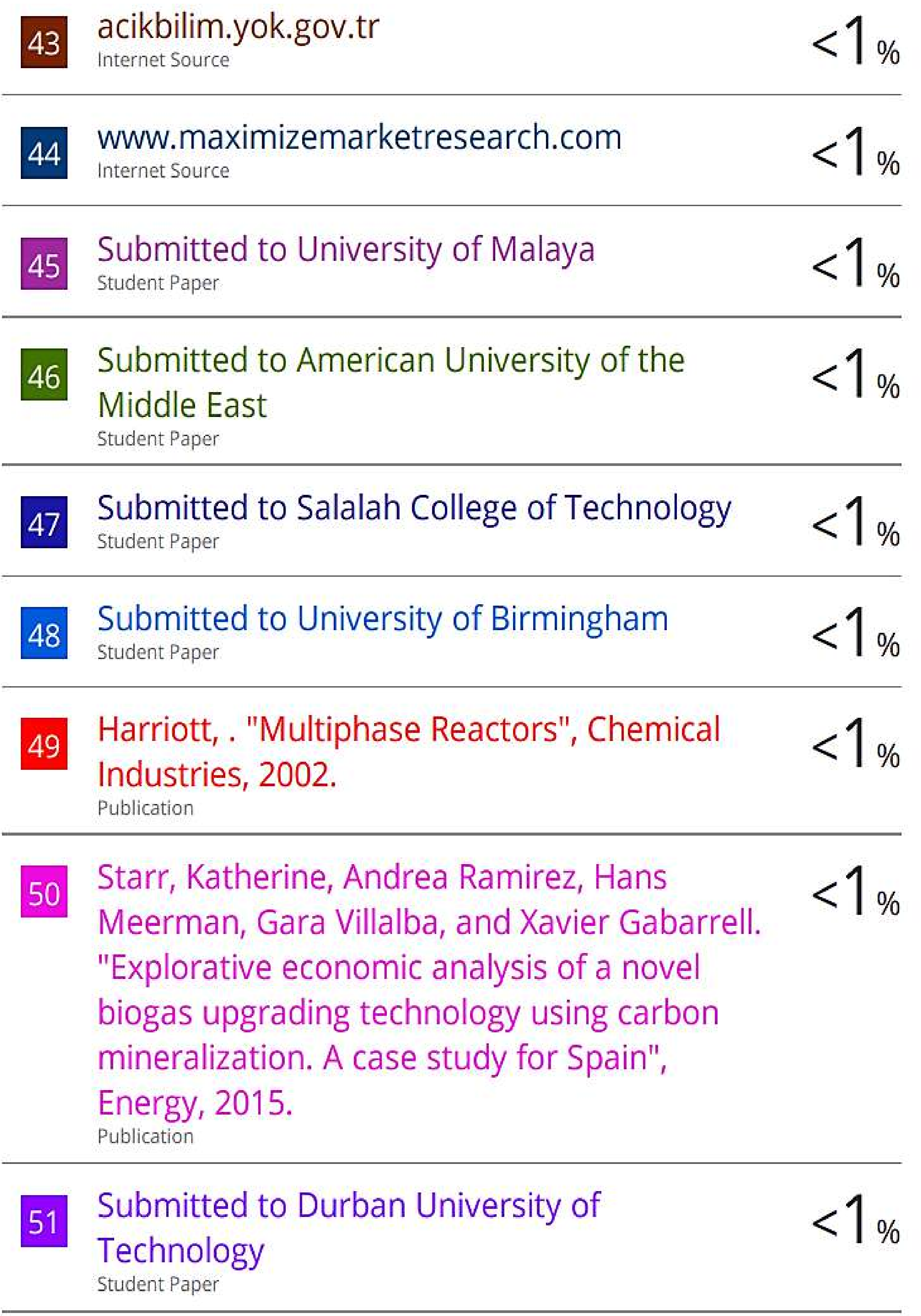

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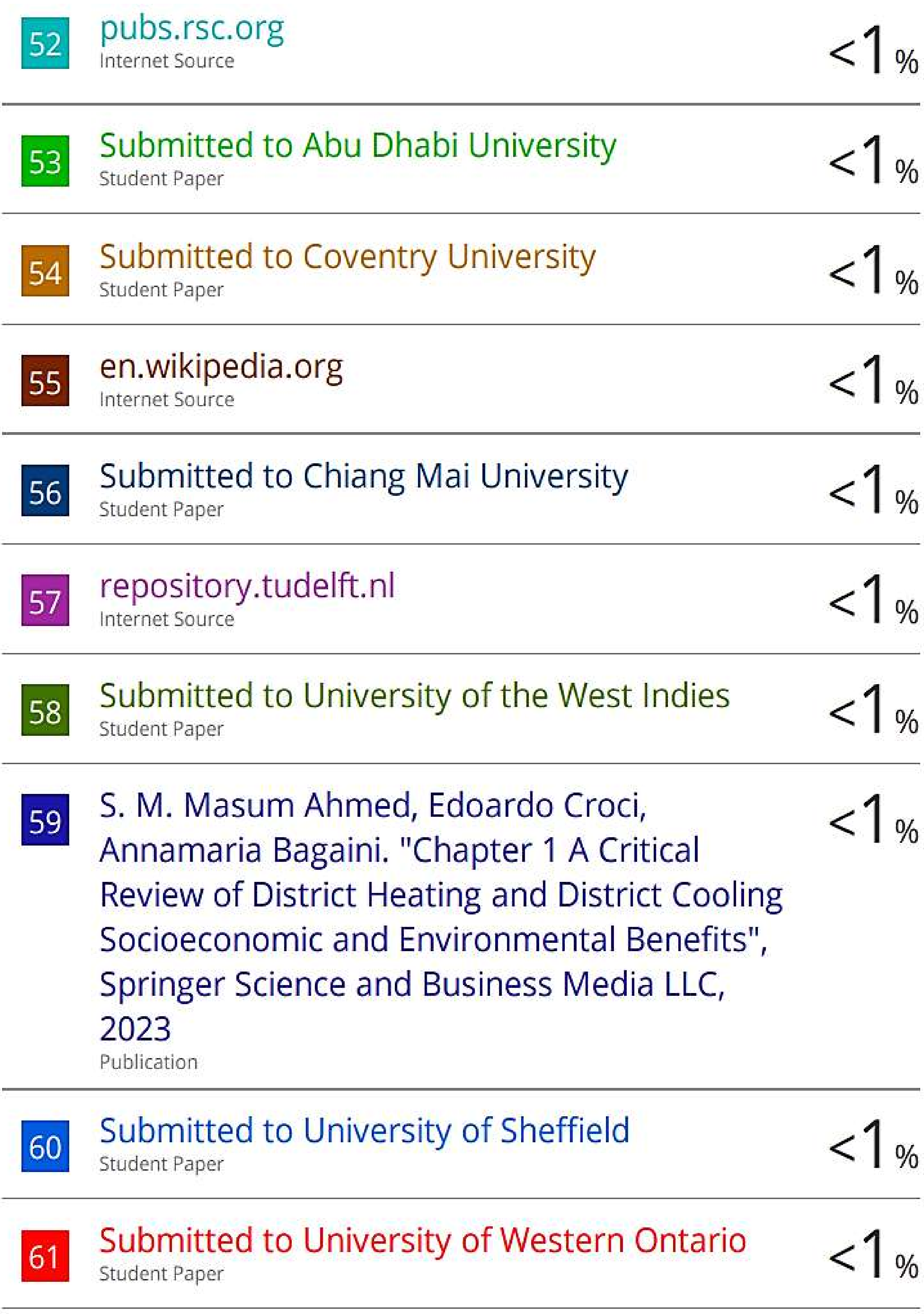

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