Design of a Portable Biogas Purification and Storage System

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DESIGN OF A PORTABLE BIOGAS PURIFICATION AND STORAGE SYSTEM

by

Anilkumar Kosna

A thesis is submitted to the Graduate College
in partial fulfillment of the requirements
for the degree of Master of Science in Engineering (Mechanical)
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Thesis Committee:

Bade Shrestha, Ph.D., Chair.
HoSung Lee, Ph.D.
Chris Cho, Ph.D.
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Anilkumar Kosna
DESIGN OF A PORTABLE BIOGAS PURIFICATION AND STORAGE SYSTEM

Anilkumar Kosna, M.S.E.
Western Michigan University, 2018

Biogas is produced from the decomposition of organic materials like manure, sewage sludge or crop fodders in anaerobic digesters. It consists mainly of 40 – 75 % of methane (CH\(_4\)), 15 – 60 % of carbon dioxide (CO\(_2\)) and trace amounts of other components. The principle constituents of biogas are similar to natural gas. Natural gas has 87 – 97 % of methane (CH\(_4\)) and 0.1 – 1 % of carbon dioxide. Natural gas is known to be an alternative fuel with a wide range of applications. The commercial purification technologies exist for large-scale biogas units. However, there are no such commercial purification technologies available for small biogas units (farm scale or household). The aim of this project is to propose a commercial portable purification and storage system for small biogas units that can be handled by a single person. This portable technology will provide an opportunity to generate an extra income source to the deprived and poor biogas unit owners, who are often located in the very poor and deprived areas where even general transportations may not available.

This work has identified and designed the components required for the proposed portable purification and storage system and their components. The proposed system has two compressors, two heat exchangers, a liquid-gas separator and a storage tank, with a total portable weight of about 12 kg excluding the storage tank. The system is capable of purifying 15 kg of biogas per hour producing and storing 4 kg biomethane. The numerical simulation of each individual component to validate the proposed purification method are also presented and discussed.
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NOMENCLATURE

\( a \) \hspace{1em} \text{fin width (}\, m\,\text{)}

\( A_p \) \hspace{1em} \text{droplet projected area (}\, m^2\,\text{)}

\( A_t \) \hspace{1em} \text{total heat transfer area (}\, m^2\,\text{)}

\( A_f \) \hspace{1em} \text{fin area (}\, m^2\,\text{)}

\( A_{\text{required}} \) \hspace{1em} \text{required area (}\, m^2\,\text{)}

\( b_1 \) \hspace{1em} \text{width of top land (}\, m\,\text{)}

\( b_2 \) \hspace{1em} \text{width of the other land (}\, m\,\text{)}

\( b_m \) \hspace{1em} \text{repulsion parameter}

\( B \) \hspace{1em} \text{bore (}\, m\,\text{)}

\( C_p \) \hspace{1em} \text{specific heat at constant pressure (}\, \frac{kJ}{kg.K}\,\text{)}

\( C_v \) \hspace{1em} \text{specific heat at constant volume (}\, \frac{kJ}{kg.K}\,\text{)}

\( C_F \) \hspace{1em} \text{correction factor}

\( C_R \) \hspace{1em} \text{compression ratio}

\( C_d \) \hspace{1em} \text{coefficient of drag}

\( d_i \) \hspace{1em} \text{inside diameter of pin (}\, m\,\text{)}

\( d_c \) \hspace{1em} \text{crank pin diameter (}\, m\,\text{)}

\( d_s \) \hspace{1em} \text{diameter of the shaft (}\, m\,\text{)}

\( d_o \) \hspace{1em} \text{outside diameter of a pin (}\, m\,\text{)}

\( D_p \) \hspace{1em} \text{droplet diameter (}\, m\,\text{)}

\( D_{V\text{min}} \) \hspace{1em} \text{minimum vessel diameter (}\, m\,\text{)}

\( D_O \) \hspace{1em} \text{outer tube diameter (}\, m\,\text{)}

\( D_{lo} \) \hspace{1em} \text{liquid outlet diameter (}\, m\,\text{)}

\( D_{go} \) \hspace{1em} \text{gas outlet diameter (}\, m\,\text{)}
E  

young’s modulus (Pa)

$F_g$  
gravity force (N)

$F_d$  
drag force (N)

FS  
safety factor

$F_b$  
bearing load (N)

$F_g$  
load by compressed gas (N)

$g$  
acceleration due to gravity ($\frac{m}{s^2}$)

$h_{\text{convective}}$  
convective heat transfer coefficient ($\frac{W}{m^2.K}$)

$H_1, H_2$  
reaction forces (N)

$I_{xx}$  
moment of inertia of the about X-axis (kg.m$^2$)

$I_{yy}$  
moment of inertia of the about Y-axis (kg.m$^2$)

$k_{ij}$  
binary interaction parameter

$k_{xx}$  
radius of gyration

$k$  
thermal conductivity ($\frac{W}{m.K}$)

$K_s$  
design parameter

$l_1$  
length of the piston (m)

$L_l$  
liquid space (m)

$L_g$  
gas space (m)

$L_C$  
length of the connecting rod (m)

$L$  
length of the piston (m)

$L_s$  
length of the piston skirt (m)

$LHV_{CH_4}$  
lower heating value ($\frac{MJ}{kg}$)

$m_a$  
mass fraction

$m$  
total mass of mixture (kg)

$m_i$  
mass of individual gas (kg)

$M_i$  
molecular weight ($\frac{kg}{kmol}$)

$mdot$  
mass flow rate ($\frac{kg}{s}$)
\( m_p \) mass of the pipe (kg)
\( m_f \) mass of the fin (kg)
\( m_{he} \) mass of heat exchanger (kg)
\( M_c \) bending moment (N.m)
\( n_r \) number of rings
\( P_d \) discharge pressure (Pa)
\( P_w \) gas pressure on cylinder walls (Pa)
\( P_b \) bearing pressure (Pa)
\( P_{allow} \) allowable pressure (Pa)
\( Pr \) Prandtl number
\( \Delta P \) pressure drop (Pa)
\( P_l \) pressure capability of liner (Pa)
\( P_{burst} \) burst pressure (Pa)
\( P_w \) working pressure (Pa)
\( P_c \) composite design pressure (Pa)
\( Q_{dis} \) heat dissipation (W)
\( r \) radius (m)
\( R \) ideal gas constant \( \left( \frac{kJ}{kg.K} \right) \)
\( R_0 \) universal gas constant \( \left( \frac{kJ}{kmol.K} \right) \)
\( Re \) Reynolds number
\( S \) stroke (m)
\( t_H \) thickness of piston head (m)
\( t_1 \) radial thickness (m)
\( t_2 \) axial thickness (m)
\( t_3 \) piston barrel thickness at open end (m)
\( t_4 \) piston barrel thickness at other end (m)
\( t \) crank web thickness (m)
\( t_v \) vessel thickness (m)
\( t_l \) liner thickness (m)

xiii
\( T_0 \) outlet temperature (K)
\( T_{inf} \) convective fluid temperature (K)
\( U_\infty \) convective fluid velocity \( (\frac{m}{s}) \)
\( V \) specific volume \( (\frac{m^3}{kg}) \)
\( V_{dot} \) volumetric flow rate \( (\frac{m^3}{s}) \)
\( V_{gmax} \) maximum gas velocity \( (\frac{m}{s}) \)
\( V_d \) displacement volume \( (m^3) \)
\( V_p \) volume of the spherical droplet \( (m^3) \)
\( V_{dotl} \) liquid volumetric flow rate \( (\frac{m^3}{s}) \)
\( V_{dotg} \) gas volumetric flow rate \( (\frac{m^3}{s}) \)
\( V_{l0} \) liquid velocity \( (\frac{m}{s}) \)
\( V_{g0} \) gas velocity \( (\frac{m}{s}) \)
\( V_{df} \) design factor
\( W_{isen} \) isentropic work (W)
\( W_r \) required work (W)
\( W_B \) buckling load (N)
\( W \) pipe length (m)
\( W_{req} \) length of the pipe required (m)
\( z_{opt} \) optimum spacing (m)

Greek symbols

\( \gamma \) specific heat ratio
\( \mu \) dynamic viscosity \( (\frac{kg}{m.s}) \)
\( \mu_o \) reference viscosity at reference temperature \( (\frac{kg}{m.s}) \)
\( \rho \) density \( (\frac{kg}{m^3}) \)
\( \omega \)  acentric factor
\( \sigma_c \)  compressive yield strength (Pa)
\( \sigma_{yield} \)  yield strength (Pa)
\( \eta \)  efficiency
\( \eta_f \)  fin efficiency
\( \eta_o \)  overall surface efficiency
\( f \)  fanning friction factor
\( \nu_d \)  design velocity (\( \frac{m}{s} \))
\( \nu \)  kinematic viscosity (\( \frac{m^2}{s} \))
1 INTRODUCTION

The population growth and fast urbanization increase the utilization of conventional energy sources based on oil, coal and natural gas, which results in an increase in energy demand as well as the environmental problems such as global warming and climate changes [1]. The energy resources of individual countries have a significant impact on its economy. The centralized energy resources in some countries raise the prices and taxes of conventional fuels. This increase in prices and taxes of conventional fuel affects the economies of developing and underdeveloped countries [2], which eventually forces to do more research on non-conventional energy sources like biomass, wind, solar, hydro and geothermal. The potential of non-conventional energy sources is enormous to support the world’s energy demand. The transition of a conventional energy-based system to non-conventional energy-based system is necessary to protect the environment and stability of the economies of countries. The contribution of non-conventional sources in present world’s energy demand is between 15 to 20 percent [3].

The developing countries of Africa, Asia, and South America are using most of the non-conventional energy supply from fuelwood for cooking and heating [4] [5]. The hydropower contributes nearly 20 percent of the global electrical power supply. The other renewable energy sources like solar energy, wind energy, bio-energy, geothermal energy, and small hydropower are contributing 2 percent of global energy demand. The present environmental policies and research studies show that the contribution of renewable sources is going to increase from 20 to 50 percent by the second half of the 21st century with the right policies in place [6]. The biomass energy is playing a key role in non-conventional energy supply. Biomass represents all the organic material (plants, trees, algae, etc.) which essentially collects and stores the sun’s energy through photosynthesis. The conversion of biomass to useful forms of energy such as heat, electricity and liquid fuels is called bioenergy or biomass energy. Bioenergy was the first energy source in human civilization, firewood has been the primary fuel for centuries. From the industrial revolution, the efficient techniques were developed to extract and burn fossil fuels, then the biomass was replaced by fuels such as oil, coal, and natural gas. Although fossil fuels replaced biomass energy, developing countries still rely on it and it is the fourth
largest source of energy with an estimate of 10 to 14 percent. Where, oil (33 percent), coal (21 percent), and natural gas (19 percent) stand as the largest primary sources of energy [6]. The United Nations intergovernmental panel on climate change (IPCC) study has explained the 21st century’s growing energy demand of the world for five scenarios. These five scenarios were developed for three different cases as follows, energy utilization of world, industrialized countries and the developing countries. Figure 1-1 depicts the dominance of biomass usage in all scenarios, the contribution of carbon-neutral biomass energy as a substitute for fossil fuel helps to meet the CO₂ targets. Biomass is not considered as a modern energy, but it has a potential to be modernized by converting solid biomass into clean and conventional energy forms such as gases, liquids, or electricity over a range of household and industrial scale.

![Figure 1-1 Commercial energy usage](image)

There are various methods available to convert biomass to useful conventional energy, some of those are direct combustion, gasification, liquid biofuels and anaerobic digestion of biomass. The Steam-Rankin technology uses the direct combustion of biomass to produce the electricity of capacity ranges 1-50 MW. However, the energy conversion efficiencies of direct biomass combustion process are low which is 10 to 15 percent. Gasification is a thermochemical process of producing combustible gas from biomass by burning it without sufficient air for full combustion, but with enough air to convert the solid biomass to gaseous fuel. The produced gaseous fuel consists of carbon monoxide, hydrogen,
carbon dioxide, nitrogen and it has a heating value of 4 to 6 MJ/Nm$^3$, which is 10 to 15 percent of the heating value of natural gas. These gases can be used in modified internal combustion engines to produce 100-200 KW with efficiencies of 15 to 25 percent [6].

Liquid biofuels play a vital role in biomass utilization. These liquid biofuels have the potential to replace petroleum-based fuels which are widely used in the transportation sector. The “biodiesel” is an important liquid fuel produced from oil-producing plants such as soybeans, palm oil trees and oilseeds like rapeseed. The compounds of biodiesel are like hydrocarbon petroleum products and the lower heating value of biodiesel is in the same range of diesel. The other potential liquid biofuels alternative to petroleum-based fuels are ethanol, methanol, and hydrogen. These are produced from crops like corn, sugarcane and from lignocellulose biomass (such as wood, straw, and grass). Finally, anaerobic digestion is a process of converting organic waste into a combustible gas called biogas. Typically, biogas consists of 60 percent of methane and 40 percent of carbon dioxide with a heating value of about 55 percent of natural gas. When it’s purified, the heating value of 1 m$^3$ purified biomethane is equal to the heating value of 0.97 m$^3$ of natural gas [2]. It shows that the purified biogas is capable to replace natural gas. Natural gas is known to be an alternative non-renewable energy source. This feature of biogas increased the interest in research and development of biogas production and purification plants.

1.1 Biogas

Biogas is a key player in the renewable energy sector. Sun et al. show that by 2020 major part of the EU-27 renewable energy is dominated by bioenergy, mostly by biogas (at least 25% share). They also predicted that the global capacity of commercial biogas is going to rise from 14.5 Gigawatts (GW) in 2012 to 29.5 GW in 2022 [7]. Biogas is produced by the decomposition of organic material like manure, sewage sludge or crop fodders in an anaerobic digester [7]. The process of degradation of organic material in an anaerobic digester is called anaerobic (without air) digestion. There are four stages of anaerobic digestion those are hydrolysis, acidogenesis, acetogenesis, and methanogenesis [2]. Biomass is a combination of complex carbohydrates, fats, and proteins. In hydrolysis, these complex carbohydrates break down to simple sugars, amino acids and fatty acids with the help of microorganisms [2]. In the acidogenesis stage, fermentative bacteria transform simple sugars and
monomeric organic compounds into organic acids, alcohols, carbon dioxide (CO₂), hydrogen (H₂) and ammonia (NH₃). The third stage is the acetogenesis, acetogenic bacteria convert products from acidogenesis stage to hydrogen (H₂), carbon dioxide (CO₂) and acetic acid (CH₃COOH). Methanogenesis is the final stage of anaerobic digestion, methanogenic bacteria convert the products of acetogenesis stage to a mixture of methane (CH₄, 50-75%), carbon dioxide (CO₂, 50-75%), varying quantities of nitrogen, hydrogen sulfide, and other components. The final product of methanogenesis is called biogas [8].

![Anaerobic digestion process diagram](image)

Figure 1-2 Anaerobic digestion process [9]
The anaerobic digestion takes place in distinct stages by various microorganisms. The favorable conditions of microorganism’s growth improve the biogas production rate [2]. The various parameters which affect the biogas production rate are pH, temperature, mixing, C/N ratio, hydraulic retention time and substrate [2]. The favorable pH range for methanogens growth is 6.7-7.5. The growth of fermentative bacteria depends on the temperature conditions; mesophilic conditions favor the fermentative bacteria growth. Mixing is a fundamental parameter of biogas generation, excess mixing stresses the microorganisms and less mixing results foam forming. The increase and decrease of the carbon-nitrogen ratio affect biogas generation, it should be of the range 16:1 – 25:1. Hydraulic retention time (HRT) is the average time the feedstock stays in the digester to transform to biogas [9]. It should be as minimum as 10-15 days.

The substrate or feedstock is the major part of biogas production. Methane content in biogas depends upon feedstock. By theory, almost all organic materials are degradable to produce biogas of various compositions of methane [2]. The major feedstock’s used in biogas production are cattle dung, pig manure, poultry waste, straw, grass silage, municipal solid waste, jatropha curcas seedcake, Pongamia pinnata seedcake, etc [10]. The biogas yield and methane content for various feedstock are shown in Table 1-1.

Table 1-1 Biogas yield and methane composition of various feedstock’s [10]

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Biogas yield (m³/kg)</th>
<th>Methane (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cattle dung</td>
<td>0.297</td>
<td>55</td>
</tr>
<tr>
<td>Pig manure</td>
<td>0.40</td>
<td>65</td>
</tr>
<tr>
<td>Poultry waste</td>
<td>0.45</td>
<td>70</td>
</tr>
<tr>
<td>Straw</td>
<td>0.341</td>
<td>51</td>
</tr>
<tr>
<td>Grass silage</td>
<td>0.576</td>
<td>52</td>
</tr>
<tr>
<td>Municipal solid waste</td>
<td>0.308</td>
<td>60</td>
</tr>
</tbody>
</table>
1.2 Biogas production

The Global bioenergy statistics 2017 reported that the global biogas production as 58.7 billion Nm$^3$. The top countries contributing biogas production are China (15.0 billion Nm$^3$), USA (8.48 billion Nm$^3$), Thailand (1.30 billion Nm$^3$), India (0.81 billion Nm$^3$), Canada (0.79 billion Nm$^3$) and EU-28 (28.9 billion Nm$^3$). EU–28 nations are dominating with the share of 49.8% whereas the production share from major continents Asia (31.9%), America (16.7%) and other continents 1.5% [11]. There are three types of biogas plants based on their sizes, those are Industrial/commercial plants, farm-scale/community plants, and household/domestic plants. The industrial/commercial biogas plants have typical capacities of >300 m$^3$. These plants are mostly installed in EU – 28 nations. Farm-scale/community biogas plants have capacities of 100 – 250 m$^3$, municipality waste is the major feedstock for these plants. These plants are dominated in Latin American nations [12]. Household/domestic biogas plants have typical sizes of 1-12 m$^3$. These plants are installed in Asian countries. The main feedstock used in these digesters is household waste whereas the industrial and community biogas plants need a centralized system to collect the feedstock and maintain the plant.

1.3 Commercial biogas plants and purification systems

The European Biogas Association (EBA) reported that the EU nations have more than 15,000 industrial/community biogas plants producing 15.0 billion m$^3$/year of biogas and more than 300 bio methane plants of production capacity 1.0 billion m$^3$/year [13]. Bio methane is the purified form of biogas. It is produced by removing carbon dioxide, hydrogen sulfide and other gases by various commercial purification process. The purification of raw biogas increases the lower heating value, compression capabilities and decreases the transportation costs. The properties of bio methane are similar to natural gas. It can be distributed to natural gas grid, used as vehicle fuel and can be efficiently used to produce electricity.

Although the composition of biogas depends on the feedstock, it mainly consists of methane (CH$_4$), carbon dioxide (CO$_2$) and small quantities of ammonia (NH$_3$), hydrogen sulfide (H$_2$S), hydrogen (H$_2$), oxygen (O$_2$), nitrogen (N$_2$), carbon monoxide (CO). The comparison of raw biogas and natural gas properties are shown in Table 1-2.
Table 1-2 Biogas composition and properties [14]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Raw biogas (vol%)</th>
<th>Natural gas (vol%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane (CH₄)</td>
<td>40 – 75 %</td>
<td>70 – 90 %</td>
</tr>
<tr>
<td>Hydrocarbons (C₂H₆, C₃H₈, C₄H₁₀)</td>
<td>...........</td>
<td>0 – 20 %</td>
</tr>
<tr>
<td>Carbon dioxide (CO₂)</td>
<td>15 – 60 %</td>
<td>0 – 8 %</td>
</tr>
<tr>
<td>Hydrogen sulfide (H₂S)</td>
<td>0.005 – 2 %</td>
<td>0 – 5 %</td>
</tr>
<tr>
<td>Oxygen (O₂)</td>
<td>0 – 1 %</td>
<td>0 – 0.2 %</td>
</tr>
<tr>
<td>Nitrogen (N₂)</td>
<td>0 – 2 %</td>
<td>0 – 5 %</td>
</tr>
<tr>
<td>Carbon monoxide (CO)</td>
<td>&lt; 0.6 %</td>
<td>0 – 4 %</td>
</tr>
<tr>
<td>Rare gases</td>
<td>...........</td>
<td>0 – 2 %</td>
</tr>
<tr>
<td>Heating value (MJ/ N m³)</td>
<td>20 – 24</td>
<td>34 – 39</td>
</tr>
<tr>
<td>Density (STP conditions)</td>
<td>1.15 kg/m³</td>
<td>0.9 kg/m³</td>
</tr>
</tbody>
</table>

The available commercial biogas purification methods are;

- Water/polyethylene glycol scrubbing
- Chemical absorption
- Pressure swing adsorption
- Membrane separation
- Cryogenic separation
1.3.1 Water/polyethylene glycol scrubbing

Water/polyethylene glycol scrubbing is a physical process, this process is based on the solubility property of CO2 and H2S in water/polyethylene. These two gases are more soluble in water/polyethylene than methane. Figure 1-3 Shows the schematic of the process. It has two main vertical cylinders used for absorption and desorption. The absorption cylinder is fed with the pressurized biogas from the bottom and water from the top simultaneously. This process is operated counter currently [15].

![Figure 1-3 Water/Polyethylene scrubbing](image)

The water which exits from the absorption cylinder is sent to the desorption/regeneration cylinder to remove CO2 and H2S. The removal of CO2 and H2S is accomplished by de-pressurizing or stripping with air. The advantages of water/polyethylene scrubbing are high efficiency (>97% CH4), simultaneous removal of H2S, capacity is adjustable by changing pressure or temperature and tolerant for impurities. The disadvantages are clogging due to bacterial growth, the possibility of foaming and low flexibility toward variation of input gas [16]. The cost of water scrubbing method is $0.16/Nm³ [15].
1.3.2 Chemical absorption/ amine scrubbing

The chemical absorption/amine scrubbing depends on the development of reversible chemical bonds between solute and solvent in an absorption cylinder. The breakage of chemical bonds takes place in the regeneration cylinder to regenerate the solvent. The aqueous solutions of mono, di, or tri ethanolamine or the aqueous solution of sodium, potassium and calcium hydroxide are used as the solvents [15]. The advantages of chemical absorption are high efficiency (>99 % CH$_4$), more CO$_2$ dissolved per unit of volume and regenerative. The main disadvantages are the expensive investments and additional chemicals required for regeneration [16]. This technique costs $0.21/Nm$^3$ [15].

![Figure 1-4 Amine scrubbing](image)

1.3.3 Pressure swing adsorption

Pressure swing adsorption is based on the property of a material to adsorb CO$_2$ gas under pressure. The materials used in pressure swing adsorption are molecular sieves of zeolite and active carbon. This process needs pretreatment step to remove H$_2$S. After the pretreatment, the biogas is sent into the pressurized adsorption column for the extraction of CO$_2$. Once the CO$_2$ is removed the methane-rich biogas is sent out of the column. The regeneration of molecular sieves is done by depressurizing the adsorption column for desorption. Figure 1-5 Shows the schematic of the typical pressure swing adsorption process. It has four vertical columns or cylinders to complete adsorption and desorption.
stages concurrently. The typical pressure and temperature of adsorption column are 7 to 8 bar and 50 to 70 °C [15]. The advantages are efficient purification (95-98% CH₄), it can be used for small capacities and tolerant to impurities. The disadvantages are expensive investment and operation and it needs costly process control [16]. The typical cost of this process is $0.49/N m³ [15].

![Figure 1-5 Pressure swing adsorption](image)

### 1.3.4 Membrane separation

The Membrane separation depends on the permeability properties of membranes for different gases. There are two basic setups available in membrane systems, they are gas-gas, and gas-liquid separation system. In gas-gas separation system, pressurized biogas (ranges from 20 to 30 bar) is pre-treated to remove H₂S, as it damages the membrane material. The membrane is made of acetate – cellulose. This system upgrades 92% methane in one step. In the gas-liquid absorption system, gaseous stream and liquid stream flows counter-currently which is separated by a microporous hydrophobic membrane. The molecules from the gaseous stream are absorbed by the liquid stream based on the permeability of various gas molecules. Generally, amine solution is used in the liquid stream. This system can purify 96% methane in one step. It costs $ 0.15/Nm³. The advantages of membrane system are a simple operation, high reliability and the capacity of small gas flow treatment. The major disadvantages are low membrane selectivity and multiple steps required to reach high purity[16].
1.3.5 Cryogenic separation

The Cryogenic separation is based on the phase change property of the matter. This process performs at high pressures (40 bars) and low temperatures (-100°C). A series of compressors and heat exchangers are used to maintain desublimation temperature of CO2. Once it reaches the required pressure and temperature the raw biogas is sent into the distillation column to separate CO2 [15]. The main advantages of cryogenic separation are the high purity of biomethane (99% CH4) and low energy required to get liquid biomethane (LBM). The disadvantages are the need of expensive investment and require high maintenance [16]. The typical cost of a cryogenic method to purify raw biogas is $0.54/Nm3.

Figure 1-6 Membrane separation

Figure 1-7 Cryogenic separation
The above discussed purification technologies are mostly used in industrial and farm-scale biogas plants. The selection of purification technology depends on energy demand (kWh/m$^3$ biomethane), purification cost ($/Nm^3$) and maintenance. Among all the purification technologies the water/polyethylene glycol scrubbing is widely used in commercial plants due to its less purification cost and maintenance.

1.4 Non-commercial/ household biogas plants

The typical capacity of household biogas plants is 1-12 m$^3$, these are mostly installed in developing countries of Asia. The legislation of those countries supports the installation of household biogas plant by providing subsidies. China and India are dominant in house hold biogas production having nearly 80% of total biogas plants. There are currently 40 million plants installed in China, whereas India has 4.5 million plants [17]. China has plans to have 80 million biogas plants by 2020 [2]. India has begun its investments on renewable energy sector by providing subsidies and incentives. The number of household biogas plants in some of the major countries are shown in table 1-3

<table>
<thead>
<tr>
<th>No.</th>
<th>Country</th>
<th>No. of plants installed</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>China</td>
<td>40 million</td>
</tr>
<tr>
<td>2.</td>
<td>India</td>
<td>4.5 million</td>
</tr>
<tr>
<td>3.</td>
<td>Nepal</td>
<td>225,000</td>
</tr>
<tr>
<td>4.</td>
<td>Vietnam</td>
<td>150,000</td>
</tr>
<tr>
<td>5.</td>
<td>Bangladesh</td>
<td>34,484</td>
</tr>
<tr>
<td>6.</td>
<td>Srilanka</td>
<td>6,000</td>
</tr>
</tbody>
</table>
There are currently more than 55 million small-scale household units operating throughout the world. The total biogas which is produced from these household units is exclusively used for cooking and lighting. At some instance, small combustion engines are used at the owner’s or producer’s house, due to the lack of commercial technology to store and transport excess biogas to the market. There is a need to develop a commercial purification and storage technology to address this problem. The successful development of portable commercial technology has a capacity to increase the economy of people who live in rural areas of developed, developing and underdeveloped countries. It can create self-employment and make people more energy independent by decentralized energy generation.

1.5 Thesis objective

The objective of this thesis is to identify, design, simulate the portable biogas purification and storage system to commercialize the small-scale biogas production. The proposed system is to design for the people who live in rural areas of underdeveloped and developing countries where no vehicle or other transportation is always available for use. The intended use of this system is for an operator to travel to biogas producers in very rural areas of a country and purchase it, then purify and store it in a tank at each biogas digester location. This imposes an important constraint on the system design that this system must be portable by one person, allowing him to travel. The weight should be the main criteria of the system design; all the components are designed in such way that the total weight of the system should not exceed 15 kg (approximate weight a normal person can carry in his/her backpack).
2 LITERATURE REVIEW

In the previous chapter, the importance of biogas in non-conventional energy resources, production, and commercial purification technologies are discussed. This chapter reviews some of the literature on portable/small biogas purification and storage system.

In 2006, Virenda K. Vijay et al., [18] developed a purification system to remove CO₂ from raw biogas of 40% CO₂ using water scrubbing method. This system comprises of single stage compressor, scrubbing column (150mm diameter and 3500mm length), water supply system, gas supply system, three-stage high-pressure compressor, and a storage cylinder. This experimental study is conducted on various flow rates of pressurized (at 1.0 MPa) water and gas ranges 1.8 – 2.0 m³/hr and 1.0 – 3.0 m³/hr respectively. This study concluded that the absorption of CO₂ in water depends on the flow rates of gas and water, the optimum 98.62 % removal of CO₂ was achieved at gas and water flow rates of 1.5 m³/hr and 1.8 m³/hr respectively.

In 2017, Aphichat Srichat et al., [19] designed a biogas purification system using chemical scrubbing method. Their focus was to study the influence of biogas flow rate, chemical solution flow rate, type of solutions and the concentration of various solutions on CH₄ enrichment. They used calcium hydroxide 0.1 mol, calcium hydroxide 0.2 mol, Mono Ethanol Amine (MEA) 0.1 mol and Mono Ethanol Amine (MEA) 0.2 mol. The biogas flow rates used in the experiment were 0.3 m³/hr, 0.6 m³/hr, and 0.9 m³/hr whereas the solution flow rates were 0.6 m³/hr, 1.2 m³/hr, 1.8 m³/hr. The test was conducted on the raw biogas of initial composition 51% methane and 39.36% carbon dioxide. The highest methane enrichment of 81.1% and 89.3% was observed with calcium hydroxide with a concentration of 0.1 and 0.2 mol at biogas and calcium hydroxide solutions flow rates of 0.3 m³/hr, 1.8 m³/hr respectively. From their experimental observations, they concluded that the greater degree of absorption is achieved with higher solution flow rate and lower biogas flow rates.

In 2017, E. Akila et al., [20] used the Pressure Swing Adsorption method for the enrichment of CH₄ in biogas. The main objective of this study is to evaluate the suitability of coconut shell derived granular activated carbon as an adsorbent to remove CO₂ at various inlet gas pressures (ranging from
0.1 to 0.8 MPa). They have used a lab scale Pressure Swing Adsorption column of 1 m height, 0.3 m diameter with a packing column space of height 0.6 m. Activated carbon layers are placed in packing column space at 0.1 m intervals. They observed that the reduction of CO₂ depends on inlet gas pressure, it increases as it reaches the optimum pressure, after that the CH₄ enrichment goes down. In this case, they have used raw biogas of 47% CO₂ and 51 % CH₄, the maximum 93.9% CH₄ content was observed at an optimum 8 bar pressure.

In 2017, Veronika Vrbova et al., [21] designed a system using a membrane separation method. This process depends on the permeability of gases in membrane materials. In this work, they used a polyimide fiber membrane, which has the permeability of 0.25, 10.7 of CH₄ and CO₂ respectively. The experiments were conducted for series and parallel connected membrane module of retentate flow 7 m³/hr. The authors concluded that the parallel connection was the most effective membrane module setup with >96% methane content whereas the series connection was around 94%.

In 2014, Abhulhassan Ali et al., [22] proposed a separation process to separate CO₂ from CH₄ using the cryogenic method. This system is based on the difference in freezing or desublimation properties of individual gases in the mixture. At an atmospheric pressure, CO₂ freezes at 194.5 K (-78.5 °C) whereas CH₄ freezes at 90.5 K (-182.5 °C). The authors designed countercurrent switched cryogenic packed beds to maintain the desublimation temperature of CO₂. The separation process involves in 3 stages, namely, packed bed surface cooling, CO₂ capture, and recovery. They studied the influence of various parameters like the flow configurations, flow rates, feed composition, cryogenic bed temperature distribution and bed saturation time on CO₂ separation. They concluded that the lower CO₂ concentration of the feed decreases the desublimation temperature, the desublimation temperature of CO₂ at 13% and 100% of constant feed flow rate of 0.3 m³/hr were identified as 169 K (-104 °C) and 190 K (-83 °C) respectively.

After detailed observation and analysis of literature on available purification technologies, it can be concluded that absorption purification methods (water/polyethylene glycol scrubbing and chemical absorption) need regeneration. The proposed system should be portable it can’t afford regeneration. Pressure swing adsorption (PSA) needs high maintenance and it required a highly skilled operator.
The proposed system is to design for the people who live in rural areas with minimal or no skilled operator. Membrane system almost works at atmospheric pressure and fouling affects its robustness.

Cryogenic method meets some of the requirements of portable biogas purification system. This process doesn’t need any regeneration because it doesn’t involve in any scrubbing (physical or chemical). The only drawback of the system is the high energy consumption, because of its requirement to maintain desublimation temperature of CO$_2$ 194.5 K (-78.5 °C). This requirement forces to have efficient heat exchangers or condensers in the system, perhaps this increases the complexity of the system. The proposed system is decided to use the condensation of CO2 instead of desublimation. The condensation of CO2 depends on the critical point; it condenses under the critical conditions. The critical pressure and temperature of carbon dioxide and methane are 7.38 MPa (1071 psia), 304.25 K (31.1 °C), 4.59 MPa (667.029 psia), and 190.41 K (-82.59 °C) respectively.
3 THERMOPHYSICAL PROPERTIES AND EQUATION OF STATE OF BIOGAS

As discussed in the previous chapter, the modified cryogenic method is decided to be used in the proposed Portable Biogas Purification Process. Thermophysical properties play a vital role in designing the cryogenic purification process as the process is based on the critical properties of gases.

Yaru S.S. et al., [23] proposed a methodology to determine the properties of a gas mixture, as follows

The mass fraction is,

\[ m_\alpha = \frac{m_i}{m} \]  \hspace{1cm} (3.1)

Specific gas constant of mixture can be estimated as,

\[ R = \sum_{i=1}^{n} R_i = \sum_{i=1}^{n} \frac{m_i}{m} \frac{R_o}{M_i} \]  \hspace{1cm} (3.2)

Specific heats at constant pressure \((C_p)\), and constant volume \((C_v)\) are [24],

\[ C_p = \sum_{i=1}^{n} \frac{m_i}{m} C_{pi} \]  \hspace{1cm} (3.3)

\[ C_v = \sum_{i=1}^{n} \frac{m_i}{m} C_{vi} \]  \hspace{1cm} (3.4)

Specific heat ratio \((\gamma)\) can be written as

\[ \gamma = \frac{C_p}{C_v} \]  \hspace{1cm} (3.5)
Although, raw biogas has traces of other constituents like Hydrogen sulfide (H₂S), Oxygen (O₂), Nitrogen (N₂) and Carbon monoxide (CO), the focus is on main constituent’s methane (CH₄) and Carbon dioxide (CO₂). The properties of pure gases are shown in Table 3-1.

Table 3-1 Properties of pure CO₂ and CH₄

<table>
<thead>
<tr>
<th>Property</th>
<th>Methane (CH₄)</th>
<th>Carbon dioxide (CO₂)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight (MW)</td>
<td>16 kg</td>
<td>44 kg</td>
</tr>
<tr>
<td>Density at STP (ρ)</td>
<td>0.668 $\frac{kg}{m^3}$</td>
<td>1.842 $\frac{kg}{m^3}$</td>
</tr>
<tr>
<td>Critical temperature (T_c)</td>
<td>190.41 K</td>
<td>304.25 K</td>
</tr>
<tr>
<td>Critical pressure (P_c)</td>
<td>4.599 MPa</td>
<td>7.384 MPa</td>
</tr>
<tr>
<td>Gas constant (R)</td>
<td>0.518 $\frac{kJ}{kg \cdot K}$</td>
<td>0.188 $\frac{kJ}{kg \cdot K}$</td>
</tr>
</tbody>
</table>

Specific heat at constant pressure and dynamic viscosity are the functions of temperature which can be calculated using empirical constants with less than 5% error. The temperature dependency of the specific heat at constant pressure is determined by,

$$C_p = A + BT + CT^2 + DT^3$$

(3.6)

Where A, B, C, D are empirical constants which are shown in Table 3-2,

Table 3-2 Empirical constants of specific heat at constant pressure

<table>
<thead>
<tr>
<th>Constant</th>
<th>Methane (CH₄)</th>
<th>Carbon dioxide (CO₂)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>4.750</td>
<td>5.316</td>
</tr>
<tr>
<td>B</td>
<td>0.6666*10⁻²</td>
<td>0.7361*10⁻²</td>
</tr>
<tr>
<td>C</td>
<td>-0.09352*10⁻⁵</td>
<td>-0.2581*10⁻⁵</td>
</tr>
<tr>
<td>D</td>
<td>-0.4510*10⁻⁹</td>
<td>0.3059*10⁻⁹</td>
</tr>
</tbody>
</table>
The dynamic viscosity is also a function of temperature which is determined by using Sutherland’s relation. This relation is based on kinetic theory of ideal gases and an idealized intermolecular-force potential [25]. The Sutherland equation is,

\[ \mu = \mu_o \left(\frac{T}{T_o}\right)^{\frac{3}{2}} \frac{T_o + S}{T + S} \]  

(3.7)

Where \( \mu_o \) is the reference viscosity at the reference temperature

\( T_o \) is the reference temperature

\( S \) is the Sutherland temperature

The constants of methane (CH\(_4\)) and carbon dioxide (CO\(_2\)) are shown below.

Table 3-3 Empirical constants of dynamic viscosity

<table>
<thead>
<tr>
<th>Constant</th>
<th>Methane (CH(_4))</th>
<th>Carbon dioxide (CO(_2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu_o ) (kg/(m * s))</td>
<td>12.01*10(^{-6})</td>
<td>13.70*10(^{-6})</td>
</tr>
<tr>
<td>( T_o ) (K)</td>
<td>273.15</td>
<td>273.15</td>
</tr>
<tr>
<td>( S ) (K)</td>
<td>197.8</td>
<td>222.2</td>
</tr>
</tbody>
</table>

The thermo-physical properties of raw biogas of 50% CO\(_2\) and 50% CH\(_4\) is computed from the individual gas properties are

Table 3-4 Properties of biogas

<table>
<thead>
<tr>
<th>Property</th>
<th>Biogas (50% CO(_2) and 50% CH(_4))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>30 kg</td>
</tr>
<tr>
<td>Density at STP (( \rho ))</td>
<td>1.529 ( \frac{kg}{m^3} )</td>
</tr>
<tr>
<td>Gas constant (R)</td>
<td>0.277 ( \frac{kJ}{kg \cdot K} )</td>
</tr>
</tbody>
</table>
Figure 3-1 to Figure 3-3 shows the specific heat at constant pressure, constant volume and the dynamic viscosity of the biogas of 50% CO₂ and 50% CH₄.

![Specific heat at constant pressure](image1)

**Figure 3-1** Specific heat at constant pressure (J/kg*K) vs temperature

![Specific heat at constant volume](image2)

**Figure 3-2** Specific heat at constant volume (J/kg*K) vs temperature
Once the thermo-physical properties of a mixture are determined, the next step is to estimate the critical properties of the mixture. The prediction of Vapor-Liquid equilibrium (VLE) is important to define the critical properties of the proposed raw biogas. There are various Equation of state (EOS) models available for pure components to predict the VLE, some of those shown in Table 3-5.

Table 3-5 Various equation of state (EOS) models

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Name</th>
<th>Equation of state</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Van der Waals (1976)</td>
<td>[ P = \frac{RT}{V-b} - \frac{a}{V^2} ]</td>
</tr>
<tr>
<td>2.</td>
<td>Redlich – Kwong (1949)</td>
<td>[ P = \frac{RT}{V-b} - \frac{a}{V(V+b)T^{0.5}} ]</td>
</tr>
</tbody>
</table>
3. Soave – Redlich – Kwong (1972) 
\[ P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)} \]

\[ P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b) + b(V-b)} \]

\[ P = \frac{RT}{V-b} - \frac{a(\theta,T)}{V(V+b) + b(V-b)} \]

\[ P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b) + c(V-b)} \]

It can be observed that a typical equation of state has two terms. The first term represents the intermolecular interactions of repulsive force and the second term represents the attraction force. The equation of state depends on the critical properties of a pure substance and empirical constants.

The Van der Waals equation of state is the simplest and oldest among all the equation of states, this equation relates the pressure (P), temperature (T), specific volume (V) and ideal gas constants (R) by the empirical constants a, b, and m. These constants can be calculated by using critical pressure (Pc), critical temperature (Tc), acentric factor (\(\omega\)) and an ideal gas constant (R). In 1949, Redlich-Kwong identified that the Van der Waals Equation is rarely accurate to predict the vapor-liquid equilibrium, they modified the Van der Waals equation by making the attraction term temperature dependent. Later, in 1972 Soave replaced the temperature dependent term with a more general temperature dependent term a(T), where,

\[ a(T) = 0.4274 \left( \frac{R^2 T_c^2}{P_c} \right) \left(1 + m \left( 1 - \left( \frac{T}{T_c} \right)^{0.5} \right) \right)^2 \]

\[ m = 0.480 + 1.57 \omega - 0.176 \omega^2 \]

\[ b = 0.08664 \frac{RT_c}{P_c} \]

In 1976, Peng-Robinson redefined the constant a(T) from Soave – Redlich – Kwong equation. The Peng – Robinson equation of state is the most popular and widely used in predicting the vapor-liquid equilibrium [26]. The Peng – Robinson (1976) equation of pure substance can be written as,
\[ P = \frac{RT}{V - b} - \frac{a(T)}{V(V + b) + b(V - b)} \]  

Where,

\[ a(T) = 0.45724 \frac{R^2 T_c^2}{P_c} (1 + k(1 - \left(\frac{T}{T_c}\right)^{0.5})^2 \]
\[ k = 0.37464 + 1.5422 \omega - 0.26922 \omega^2 \]
\[ b = 0.07780 \frac{RT_c}{P_c} \]

Figures 3-4 & 3-5 shows the P-V diagram of Pure CO\textsubscript{2} and CH\textsubscript{4} from the Peng-Robinson equation of state. An isotherm of various temperatures is plotted on a P-V diagram to study the phase transformation of the substances. The Figures 3-4 & 3-5 illustrates at the critical pressure the slope of isotherm is zero, the temperature and specific volume at the critical pressure are called as the critical temperature and the critical specific volume. The point is called the critical point, this point distinguishes the phases. At the critical point, the liquid and vapor phases co-exist in equilibrium. The co-existence of vapor-liquid equilibrium is represented by the spinodal curve. The spinodal curve provides the information of fluid at its saturation liquid state (left part of the curve) and at its saturated vapor state (right part of the curve). The critical point makes the boundary between saturated liquid and vapor phase. The region at top right of the spinodal curve is distinguished as the super-heated vapor region, left side as the compressed liquid region, and the region under the spinodal curve is saturated vapor-liquid region. The critical point obtained from the Peng – Robinson equation of state is in good agreement with the tabulated critical point by less than 1% error.
The information extracted from the above P-V diagrams is useful for the proposed cryogenic purification system, but it doesn’t provide enough information to define the thermodynamic states of system as the proposed system involves CO₂ – CH₄ mixture. Gang Xu et al. [27] studied the effect of various critical states of pure gases on its mixture critical point. They concluded that lower critical state of substances lowers the critical state of higher critical state substances. For the proposed system the lower critical state substance is CH₄ at 190.41 K (-82.8 °C) of the critical temperature and 4.599 MPa (665 psia) of the critical pressure. This lower critical state of CH₄ influences the CO₂ critical state from 304.25 K (31.25 °C), 7.384 MPa (1071 psi) to some other point.

An equation of state is developed from the available resources to quantify the influence of CH₄ composition in the critical state of CO₂ – CH₄ binary mixture. Peng – Robinson equation of state of a pure substance can be extended to the binary mixture by selecting the proper mixing rule. Among all the mixing rules, Van der Waals mixing rules are widely used in process simulation. Seif – Eddeen K. Fatten et. al. [26] proposed a methodology to apply Van der Waals mixing rules to Peng-Robinson equation of state. In their work, they proposed a Semi-empirical correlation for binary interaction parameters of CH₄ – CO₂ mixture to minimize the deviation of vapor-liquid equilibrium (VLE) prediction from the experimental predictions. The equations used to develop an equation of state of carbon dioxide in a CO₂-CH₄ binary mixture is as follows.
The Peng–Robinson equation of state of mixture can be written as,

\[
P = \frac{RT}{(V - b_m)} - \frac{\alpha_m(T)}{V(V + b_m) + b(V - b_m)}
\]  

(3.9)

The attraction parameter \( \alpha_m(T) \) can be expressed as,

\[
\alpha_m(T) = \sum_{i=1}^{2} \sum_{j=1}^{2} x_ix_j (1 - k_{ij})\sqrt{a_i a_j}
\]

The repulsion parameter \( b_m \) as,

\[
b_m = \sum_{i=1}^{2} x_i b_i
\]

Binary interaction parameter \( k_{ij} \) can be written as,

\[
k_{ij} = \frac{1}{2} \frac{b_j}{b_i} \sqrt{\frac{a_i}{a_j}} - \frac{1}{2} \frac{b_i}{b_j} \sqrt{\frac{a_j}{a_i}} + \frac{1}{2} \frac{b_jRT}{\sqrt{a_i a_j}} \frac{\theta_1}{T_{c,i} \theta_2}
\]

Where,

\( x \) is a mole fraction.

\( a, \) and \( b \) are the attraction and repulsion terms of pure components.

\( \theta_1 = 2.5522, \) and \( \theta_2 = 0.80726 \) are the empirical constants of the methane/carbon dioxide mixture[26].

Figure 3-6 shows the P -V diagram of 50% CO\(_2\) – 50% CH\(_4\) binary mixture from the modified Peng – Robinson equation of state. It illustrates that the critical state of CO\(_2\) – CH\(_4\) mixture is at 255 K (-18°C), 4.82 MPa (699.08 psia), and 0.0045 m\(^3\)/kg. This explains that for a given mixture the vapor-liquid equilibrium of CO\(_2\) co-exists at the critical point.
Figure 3-6 P – V diagram of 50% methane and 50% carbon dioxide mixture

It can also be concluded that the composition of CH₄ – CO₂ binary mixture and respective critical states are important for the design. Figures 3-7, 3-8 & 3-9 show the critical temperature, pressure, and specific volume as a function of CO₂ composition extracted from the equation of state of CO₂ – CH₄ binary mixture.

Figure 3-7 Critical temperature vs CO₂ mole fraction
Figure 3-8 Critical pressure vs CO₂ mole fraction

Figure 3-9 Critical specific volume vs CO₂ mole fraction
4 EXPERIMENTAL VALIDATION OF EQUATION OF STATE OF BIOGAS

4.1 Experiment setup

The proposed equation of state successfully quantifies the critical states for variable compositions of CO₂ – CH₄ binary mixture. An experiment is necessary to validate the equation of state of CO₂ – CH₄ mixture to use it in proposed purification process design. The typical equation of state defines the relation between the state variables pressure (P), temperature (T), and specific volume (v). These state variables are dependent on each other, for a closed system the variation of pressure and temperature is independent of the specific volume, this simplifies the variables as pressure and temperature. The experiment is designed as a closed system to record the pressure and temperature at constant specific volume. This pressure and temperature data can be used to validate the proposed equation of state by comparing the theoretical and experimental pressure and temperature data. A layout schematic of the experimental setup is shown in Figure 4-1, with a detailed explanation of each component in the following sections.

![Layout schematic of the experiment setup](image)

Figure 4-1 Layout schematic of the experiment setup
4.1.1 Gas mixing equipment

The Gas mixing equipment is the primary component of the system it prepares the CO₂-CH₄ binary mixture of specified compositions. It comprises of volumetric flow controllers, pressure gauges, thermocouples, and a gas mixer as shown in figure 4-2. The volumetric flow controllers are used to prepare variable compositions of homogeneous CO₂ – CH₄ binary mixture by controlling the volumetric flow of individual gases based on the given volume fractions. Omega FL4217 – V Acrylic rotameters of maximum flow capacity of 100 SCFH (2.832 m³/hr) is used as a flow controller. The operation of rotameter is based on the variable area principle in which the fluid flow raises a float in a tapered tube. The higher the flow, greater the float height is observed. The flow rate is directly proportional to the height of the float. These are typically designed for air but these can also use for other fluids by using the correction factor. The correction factor is shown below.

\[
CF = \sqrt{\frac{(SG)(T_{0})(14.7)}{(1.0)(P_{0})(530)}}
\]  
(4.1)

Where, SG is the specific gravity of the gas, \(T_{0}\), \(P_{0}\) are the operating pressure and temperatures then the volumetric and mass flow rate of the incoming gas is calculated from the measured flow rate as.

\[
V_{dot} = V_{dot_{measured}} CF  \quad \quad \quad m_{dot} = \frac{P_{0}V_{dot}}{R T_{0}}
\]  
(4.2)

Figure 4-2 Gas mixing equipment

1) CH₄ flow controller, 2) CO₂ flow controller, 3) Mixture flow controller, 4) Thermocouple, 5) Pressure gauge, 6) Gas mixer.
4.1.2 Accumulator

An accumulator is a flow storage device used to store the potential energy through the compression of the gas. It is placed after the mixing equipment, the objective of this accumulator is to hold/control the gas mixture flow to prevent load on the compressor. Figure 4-3 shows the accumulator used in this system, accumulator outlet is connected to a needle valve (to control/stop the flow) and a gas filter (filter unwanted dust particles).

![Accumulator Diagram](image)

Figure 4-3 Accumulator
1) Mixture Inlet, 2) Accumulator, 3) Needle valve, 4) Gas filter, 5) Mixture Outlet.

4.1.3 Reciprocating compressor

The reciprocating compressor is an important component of the system. The specifications of this component greatly influence the experiment procedure. Figure 4-4 shows the two-stage reciprocating compressor used in the experiment. This multi-stage compressor takes the gas in and compresses it to the desired outlet set pressure. The pressure regulator is used to set/adjust the discharge pressure. This compressor is also equipped with water cooling for stage two to maintain relatively low outlet temperature.
Figure 4-4 Multi-stage reciprocating compressor

1) Gas inlet, 2) Gas outlet, 3) Pressure Regulator, 4) Thermocouple, 5) Crankcase, 6) Stage 1 compression chamber, 7) Stage 2 compression chamber, 8) water cooling lines.

The specifications of the compressor are,

Table 4-1 Specifications of commercial compressor

<table>
<thead>
<tr>
<th>Manufacturer</th>
<th>Young Heng</th>
</tr>
</thead>
<tbody>
<tr>
<td>Working pressure</td>
<td>30 MPa</td>
</tr>
<tr>
<td>Voltage</td>
<td>110 V</td>
</tr>
<tr>
<td>Motor power</td>
<td>1.8 kW</td>
</tr>
<tr>
<td>Net weight</td>
<td>16.2 kg</td>
</tr>
<tr>
<td>Maximum flow capacity</td>
<td>50 L/min (3 m³/hr)</td>
</tr>
</tbody>
</table>

4.1.4 Liquid – Gas Separator

The objective of Liquid – Gas separator is to separate the liquid from the gas. In this experiment, it is used to store the pressurized gas mixture to record pressure and temperature at constant volume. Figure 4-5 shows the liquid-gas separator used in this experiment, both the liquid and gas outlets were closed.
by ball valves to make it a closed system. It also shows the location of pressure gauge and thermocouples.

Figure 4-5 Liquid – Gas Separator

1) Mixture inlet, 2) Thermocouple, 3) Pressure gauge, 4) Gas outlet valve, 5) Liquid – Gas separator 6) Liquid outlet valve.

The specifications of Liquid-Gas separator are,

Table 4-2 Specifications of Liquid-Gas separator

<table>
<thead>
<tr>
<th>Manufacturer</th>
<th>Didion Separator Company</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td>3.2 in (0.081 m)</td>
</tr>
<tr>
<td>Height</td>
<td>11.5 in (0.292 mm)</td>
</tr>
<tr>
<td>Volume</td>
<td>1.516 L (1.516 × 10⁻³ m³)</td>
</tr>
<tr>
<td>Tare weight</td>
<td>1.316 kg</td>
</tr>
<tr>
<td>Operating pressure</td>
<td>12.4 MPa</td>
</tr>
</tbody>
</table>

4.1.5 Cooling system

The cooling system is the most important and complicated component in the entire experimental setup. The proposed equation of state indicates very low critical temperatures to transform gaseous CO₂ into
liquid CO\(_2\). Figure 3 – 7 shows the influence of CH\(_4\) composition on critical temperature of CO\(_2\). For 50 % methane and 50% carbon dioxide the critical pressure and temperatures are at 4.82 MPa (699.08 psia), 255 K (-18 °C) respectively. The cooling system needs to maintain this low temperature to condensate CO\(_2\). Typical commercial heat exchangers are not adequate to provide such a low temperature. Dry ice was decided to use in the system to provide the required cooling.

**4.1.6 Data acquisition system**

As discussed in previous sections the experiment is aimed to record the pressure and temperature at constant specific volume. The digital pressure gauge is used to record the pressure variation in the liquid-gas separator. This pressure gauge can measure up to 34.47 MPa with +/- 1 % accuracy. Figure 4-6 (a) shows the digital pressure gauge used in the experiment. Omega TC-K-NPT-G-72 Thermocouples are used to measure the temperature at different locations of the experiment. A thermocouple is a device which produces a temperature – dependent voltage as a result of temperature difference at the junction. The voltage signals are transmitted to the DAQ system, which is then transferred to LabVIEW VI to convert the analog signal to digital code. Figure 4-6 (b) shows the thermocouples used in the experiment. The specific volume of the fluid is the volume occupied by one kilogram of fluid, which can be determined by measuring the total mass of the fluid in the tank. Adam CBK 35a-USB Bench-Scale was used to measure the fluid mass in the tank, this can measure up to 16 kg with 0.5 g readability.

![Digital pressure gauge](image1.png)
![K-type thermocouple](image2.png)
![Bench-Scale](image3.png)

Figure 4-6 Data acquisition equipment
4.2 Experimental procedure

Before starting the system, it is important to close all the valves. Initially, valves of pure gas tanks (CH₄ and CO₂) are opened to reach the proper pressure and flow rate throughout the gas mixing system. Once the pure gases are released into the gas mixing system, the flow meters are manually adjusted to specified flow rates based on the required volume fractions of the binary mixture. The binary mixture from the gas mixing system is then sent to an accumulator to build the inlet pressure for the compressor. This accumulator is operated with the needle valve to control the flow of mixture.

The compressor is set to an operating pressure of the Liquid-Gas separator to store the gas mixture. The compressor is then turned on and left for 4 to 5 seconds to build the suction pressure in the compressor. The valve of an accumulator is opened to allow the gas mixture to the compressor inlet. Once the liquid-gas separator reaches the adjusted pressure, the compressor automatically shuts off. The variation of pressure and temperatures at various locations are recorded. The experiment was performed for Pure CO₂, 80% CO₂ – 20% CH₄ mixture, and 50% CO₂ – 50% CH₄. The inputs required for the gas mixing equipment is shown below.

<table>
<thead>
<tr>
<th>S.no.</th>
<th>XCO₂</th>
<th>XCH₄</th>
<th>VdotCO₂ $\frac{m^3}{hr}$</th>
<th>VdotCH₄ $\frac{m^3}{hr}$</th>
<th>Vdotmixture $\frac{m^3}{hr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>1</td>
<td>0</td>
<td>1.98</td>
<td>0</td>
<td>1.98</td>
</tr>
<tr>
<td>2.</td>
<td>0.8</td>
<td>0.2</td>
<td>1.58</td>
<td>0.39</td>
<td>1.98</td>
</tr>
<tr>
<td>3.</td>
<td>0.5</td>
<td>0.5</td>
<td>0.99</td>
<td>0.99</td>
<td>1.98</td>
</tr>
</tbody>
</table>

4.3 Validation of equation of state of CO₂ – CH₄ binary mixture

The validation of the equation of state of CO₂ – CH₄ binary mixture is achieved by comparing the theoretical and experimental saturated vapor pressure and temperature at constant specific volume. As
discussed in the experimental procedure, all mixtures are compressed to 12.4 MPa (operating pressure of liquid –gas separator tank) and then cooled to saturated vapor temperature (obtained from the equation of state of binary mixture) to determine the saturated vapor pressure at constant volume experimentally.

![Pressure rise Vs Time](image1)

Figure 4-7 Pressure rise vs time

![Temperature rise Vs Time](image2)

Figure 4-8 Temperature rise vs time

Figures 4-7 & 4-8 show the pressure and temperature rise of various binary mixtures due to the compression. It illustrates that the pressure and temperature are interdependent variables when
pressure increases the temperature also increases, and vice versa. It can be observed that the compression time of the gases varies based on the gas composition, the compression time of pure CO$_2$, 80% CO$_2$, and 50% CO$_2$ are 25.5 min, 12 min, and 8 min, respectively. This compression time indicates that the heavier molecules require more energy for compression. Although all mixtures are stored in the same tank at the same pressure. The mass of fluid stored in the tank varies from mixture to mixture because of the dissimilar molecular weight of the mixture. Once the compression is completed, all the valves of Liquid – Gas Separator tank are closed to make it a closed system. The properties of the fluid mixture after the compression are shown in Table 4-3.

Table 4-4 Properties of fluid after compression

<table>
<thead>
<tr>
<th>Mixture</th>
<th>$m_{\text{mixture}}$ (kg)</th>
<th>$m_{\text{CO}_2}$ (kg)</th>
<th>$m_{\text{CH}_4}$ (kg)</th>
<th>$\nu_{\text{mixture}} \left( \frac{m^3}{kg} \right)$</th>
<th>P (MPa)</th>
<th>T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure CO$_2$</td>
<td>--------------</td>
<td>0.532</td>
<td>------------</td>
<td>2.846 $\times$ $10^{-3}$</td>
<td>12.49</td>
<td>318.41</td>
</tr>
<tr>
<td>80% CO$_2$</td>
<td>0.280</td>
<td>0.257</td>
<td>0.023</td>
<td>5.403 $\times$ $10^{-3}$</td>
<td>12.50</td>
<td>302.43</td>
</tr>
<tr>
<td>50% CO$_2$</td>
<td>0.173</td>
<td>0.127</td>
<td>0.046</td>
<td>8.761 $\times$ $10^{-3}$</td>
<td>12.51</td>
<td>299.17</td>
</tr>
</tbody>
</table>

The saturated vapor properties of the mixtures at specified specific volume is obtained from the equation of state of binary mixture is shown in table 4-4.

Table 4-5 Saturated vapor properties of the mixtures at specified specific volume

<table>
<thead>
<tr>
<th>Mixture</th>
<th>Saturated vapor temperature (K)</th>
<th>Saturated vapor pressure of CO$_2$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure CO$_2$</td>
<td>301</td>
<td>6.91</td>
</tr>
<tr>
<td>80% CO$_2$</td>
<td>261</td>
<td>3.96</td>
</tr>
<tr>
<td>50% CO$_2$</td>
<td>224</td>
<td>2.83</td>
</tr>
</tbody>
</table>

Once the saturated vapor temperatures are identified, the next step is to maintain the saturated vapor temperature to record the saturated vapor pressure of mixture experimentally. The experimental saturated vapor pressure is compared to the theoretical saturated vapor pressure to validate the equation of state of binary mixture. The required saturated temperature of pure CO$_2$ is 301 K; this temperature is greater than the ambient air temperature (295 K). So, the natural convection of ambient air is enough
to dissipate heat from the storage tank. On the other hand, the mixture saturated vapor temperature is less than the ambient temperature, the natural convection alone cannot achieve the required temperature drop therefore an external cooling (provided by dry ice) is used to attain the required low saturated vapor temperatures. Dry ice is the solid form of CO$_2$, it sublimes at 194.65 K (-78.5 °C ), at atmospheric pressure. When the tank is covered with dry ice the sublimation process cools the tank up to 218 K (-55°C) which essentially cools the gas mixture to required temperature.

![Pressure drop Vs Temperature (Pure CO2)](image1)

![Pressure drop Vs Temperature (80% CO2)](image2)

![Pressure drop Vs Temperature (50% CO2)](image3)

Figure 4-9 shows the pressure drop with respect to the temperature, pressure of a mixture at saturated vapor temperature is compared to theoretical saturated vapor pressure to validate the proposed equation of state. The error percentage of the validation is calculated as.
\[ Error \% = \left| \frac{P_{\text{exp}} - P_{\text{the}}}{P_{\text{exp}}} \right| \times 100 \] (4.3)

Table 4-5 shows the comparison of experimental saturated vapor pressure with the theoretical vapor pressure at saturated vapor temperature and specific volume.

Table 4-6 Comparison of theoretical and experimental saturated pressures

<table>
<thead>
<tr>
<th>Mixture</th>
<th>( T_{\text{saturated}} )</th>
<th>( P_{\text{saturated}} ) (theoretical)</th>
<th>( P_{\text{saturated}} ) (Experimental)</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure CO(_2)</td>
<td>301</td>
<td>6.91</td>
<td>7.16</td>
<td>3.49</td>
</tr>
<tr>
<td>80% CO(_2)</td>
<td>261</td>
<td>3.96</td>
<td>4.94</td>
<td>19.83</td>
</tr>
<tr>
<td>50% CO(_2)</td>
<td>224</td>
<td>2.83</td>
<td>3.87</td>
<td>26.63</td>
</tr>
</tbody>
</table>

The experimental saturated pressure of pure CO\(_2\) at the saturated temperature and specific volume is in good agreement with the theoretical saturated pressure. The error percentage is calculated as 3.49%. The error percentage of 80% CO\(_2\) and 50% CO\(_2\) is determined as 19.83%, 26.63% respectively. This higher error percentage in mixtures is caused mainly due to the lower saturated temperature and the cooling system used for it. As discussed earlier, dry ice was used to maintain the lower temperatures. This dry ice rapidly cools the liquid-gas storage tank to temperatures up to 218 K. This rapid cooling causes errors in data acquisition, which essentially lead to a higher error percentage. Although the higher error percentage is observed, this error is consistent with the saturated temperature. This error can be corrected by incorporating a better cooling system.
5 PURIFICATION PROCESS AND COMPONENTS DESIGN

5.1 Purification process design

The operating principle for the proposed system is to compress and cool the biogas until the carbon dioxide changes its phase from gas to liquid. The liquid CO2 and the gaseous methane will then be separated and stored in their respective tanks. For the preliminary design, the composition of raw biogas is assumed to be comprised of 50% methane (CH4), and 50% carbon dioxide (CO2). From the Figure 5-1, a condensation point is chosen in the liquid region of 50% CO2 – 50% CH4 mixture. The temperature and pressure of chosen condensation point are 206 K (-67 °C), 5.65 MPa (819.46 psi) respectively. The chosen point is in the liquid region for all the compositions of CO2 – CH4 binary mixture.

![Figure 5-1 Equation of state of CO2 of CO2 – CH4 binary mixture](image)

Figure 5-1 Equation of state of CO2 of CO2 – CH4 binary mixture
For this portable purification system, size and weight are of highest priority. The important design parameter which decides the weight of the system is the mass flow rate. All the components have been designed to meet the goal of 4 kg methane processed in about 1 hour which leads to the total mass flow rate of raw biogas to be 15 kilograms per hour. 4 kg of methane is chosen based on the availability and usage of a small propane tank, currently in the market. The identification of the thermodynamic states of the system plays a crucial role in component design. The thermodynamic processes of the proposed system are shown in Figure 5-2.

Figure 5-2 Portable biogas purification system design

The Ideal thermodynamic processes required for the purification process are

1-2 Compression process
2-4 Isobaric Heat rejection process (by air and liquid CO₂ expansion)
4-5 Liquid – Gas separation process (by gravity separation)
5-6 Compression process
5.1.1 Process 1-2 compression

In this process, raw biogas (50% CH₄ and 50% CO₂) of 15 kg/hr enters into the compression system at ambient conditions (0.1 MPa, 300 K), which is then compressed around the liquefaction pressure (5.65 MPa). The following isentropic relations are used to calculate the required compression ratio, power and outlet temperature.

\[
\frac{V_1}{V_2} = \left(\frac{P_2}{P_1}\right)^{\frac{1}{\gamma}} \quad (5.1)
\]

\[
\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}} \quad (5.2)
\]

\[
W_{isen} = \frac{mdot \gamma R_{bio} (T_2 - T_1)}{1 - \gamma} \quad (5.3)
\]

\[
W_{req} = \frac{W_{isen}}{\eta} \quad (5.4)
\]

Where \(\gamma\) is the specific heat ratio, which depends on the temperature. All these isentropic values are corrected by applying the compressor efficiency coefficient of 80%. The corrected pressure, temperature and required power of the biogas exit from the compressor are 5.65 MPa (820 psia), 908.68 K (635.68 °C) and 3.82 kW respectively.

5.1.2 Process 2-4 isobaric heat rejection

The objective of this system is to cool the compressed biogas from 908.68 K to liquefaction temperature (206 K). The overall heat dissipation required for this temperature drop is 4.43 kW. Single heat exchanger alone cannot achieve this temperature drop using ambient air as a convective fluid. So, the heat rejection system is retrofitted by an extra heat exchanger. This extra heat exchanger is proposed to use the liquid CO₂ coming out from the liquid-gas separator by expanding it from
liquefaction pressure (5.65) to ambient pressure (1 bar). This expansion leads to the temperature drop from critical temperature (216 K) to 156.91 K, this can be calculated using isentropic relation. In order to define heat dissipation required from the first heat exchanger which is dependent on expanded liquid CO2 outlet temperature, an iterative program is developed to study and calculate the impact of expanded liquid CO2 temperature on biogas outlet temperature from heat exchanger 1. After some iterations, the outlet biogas temperature of the heat exchanger 1 is determined as 375.41 K by maintaining the inlet air coolant temperature at 300 K, inlet expanded CO2 coolant temperature at 156.91 K and the outlet biogas temperature from heat exchanger 2 at 207.33 K (Critical temperature). The major thermodynamic equations used to develop the iterative program are explained below.

The required heat dissipation equation from the first law of thermodynamics by neglecting kinetic energy, potential energy, and work done on the system.

\[ Q_{dis} = \dot{m} C_p \Delta T_{bio} \]  \hspace{1cm} (5.5)

The required heat transfer surface area is calculated by replacing the required heat dissipation by Newton’s law of cooling.

\[ h_{coolent} A_{required} \Delta T_{coolent} = \dot{m} C_p \Delta T_{bio} \] \hspace{1cm} (5.6)

\[ A_{required} = \frac{\dot{m} C_p \Delta T_{bio}}{h_{coolent} A_{required} \Delta T_{coolent}} \] \hspace{1cm} (5.7)

5.1.3 Process 4-5 liquid – gas separation

After the heat – rejection system, the biogas reaches under the critical properties of carbon dioxide (5.16 MPa, 216 K). At this state, the entire gaseous CO2 converts to liquid based on the proposed biogas equation of state. The process uses gravity separation method to separate liquid CO2 from gaseous CH4. There are two approaches to sizing the gravity separation system which is as follows, The Sounders – Brown approach and the droplet settling theory. Sounders – Brown approach
determines the maximum gas velocity by balancing the forces on liquid droplet (drag force in upward direction exerted by gas and gravitation pull exerted by liquid droplet in the downward direction). The required minimum diameter is calculated based on the maximum gas velocity. The equations are as follow

\[
V_{\text{gmax}} = \sqrt{\frac{4gD_p \left( \rho_l - \rho_g \right)}{3C_d \rho_g}} \quad (5.8)
\]
\[
D_{V\text{min}} = \sqrt{\frac{4V_{\text{dot}g}}{\pi V_g}} \quad (5.9)
\]

The separation process is assumed to be an isothermal and isobaric process. The selection of separator geometry is important for the system. The vessel has a liquid and gas outlet. For an ideal separation, the mass flow rate of the liquid CO\textsubscript{2} which exits from the liquid outlet is 11 kg/hr whereas the mass flow rate of the gaseous methane which exits from the gas outlet is 4 kg/hr. The liquid CO\textsubscript{2} is directed towards the expansion valve to expand it from 5.16 MPa (750 psia) to 0.1 MPa (14.50 psia). This expansion leads the temperature drop from 216 K (57 °C) to 156.91 K (116.09 °C). Which is then used as a coolant for the heat exchanger 2.

5.1.4 Process 5-6 isentropic compression process

The pure methane which exits from the gas outlet is sent to further compression, to store it in CNG quality. Typically, in United States CNG (Compressed natural gas) is stored approximately around 20 MPa pressure. The pure methane is compressed from 5.16 MPa to 22.06 MPa. The final properties of biomethane stored in storage cylinder are 22.06 MPa (3200 psia) and 316.3 K (43.31 °C).

5.1.5 Efficiency of the purification system

The ratio of actual work required for the entire system to lower heating value of biomethane determines the efficiency of the system. Figure 5-2 identifies the required components of the purification system,
those are compressor 1, heat exchanger 1, heat exchanger 2, liquid-gas separator, compressor 2 and light-weight storage tank. The power required by the work consuming devices are 3.82 kW (Compressor 1), 0.141 kW (Compressor 2) and 23 W (Fan). The lower heating value of the biomethane is assumed to be equal to pure methane which is 50 * 10^6 J/kg. The efficiency of the system is calculated by,

\[ \eta = \frac{W_{\text{required per kg}}}{LHV_{CH_4}} \times 100 \]  

(5.10)

It can be concluded that the 7% of pure methane’s energy is consumed to purify the biogas of 15 kg/hr of 50% methane and 50% carbon dioxide.

The major components of the proposed system are identified as Compressors, Heat Exchangers, Liquid – Gas Separator and Gas Storage Cylinder. The following sections discuss the Selection, Design and Numerical Analysis of individual components based on process requirements.

5.2 Compressor design and finite element analysis

The goal of this section is to design the compressor for the proposed system. The proposed purification system requires two compressors to maintain the required pressure. From figure 3-9, it can be observed that the compressor 1 needs to compress the biogas from ambient pressure (0.101 MPa) to critical pressure of CO$_2$ (5.16 MPa) whereas, the compressor 2 is used to compress the biomethane (4 kg/hr) from critical pressure of CO$_2$ to CNG quality (22 MPa). The required compression ratios of compressor 1 and 2 are 21.713, 3.03 respectively. The compressor inlet parameters are shown in Table 5-1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Compressor 1</th>
<th>Compressor 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate ($m_{\text{dot}}$)</td>
<td>15 kg/hr (Biogas)</td>
<td>4 kg/hr (Biomethane)</td>
</tr>
<tr>
<td>Suction pressure ($P_s$)</td>
<td>0.101 MPa (ambient)</td>
<td>5.16 MPa</td>
</tr>
<tr>
<td>Suction temperature ($T_s$)</td>
<td>300 K</td>
<td>206.38 K</td>
</tr>
</tbody>
</table>

Table 5-1 Input parameters of compressors
<table>
<thead>
<tr>
<th>Required compression ratio (CR)</th>
<th>21.71</th>
<th>3.03</th>
</tr>
</thead>
<tbody>
<tr>
<td>Required discharge pressure (P\text{d})</td>
<td>5.65 MPa</td>
<td>22.06 MPa</td>
</tr>
<tr>
<td>Isentropic discharge temperature (T\text{d})</td>
<td>908.68 K</td>
<td>316.31 K</td>
</tr>
<tr>
<td>Required power (W\text{req})</td>
<td>3.82 kW</td>
<td>0.141 kW</td>
</tr>
</tbody>
</table>

An appropriate selection of compressor type is important for the system. An ideal compressor is to flexible to change the inlet gas flow rate (if required), light-weight, cost-effective, and robust. Figure 5-3 summarizes the available compressor types. Although various kinds of compressors are available, each one of it has its own advantages and disadvantages. The thermal compressor is a type of ejector, that uses a high-pressure gas jet to pressurize the incoming gas by mixing. These type of compressors has no moving parts. But, the gas mixing leads to low operating pressure ranges. Dynamic compressors use the centrifugal or axial force to increase the velocity of the fluid and then converts the velocity to pressure by restricting the flow. These compressors are further divided into centrifugal (uses Centrifugal force) and axial (uses axial force) compressors. They can provide continuous flow but, it can only be applicable for low-pressure differences.

![Figure 5-3 Types of compressors](image)

The positive displacement compressors increase the incoming gas pressure by reducing the volume. The two main types of positive displacement compressors are rotary and reciprocating. The rotary compressor uses a set of screws, lobes, or vanes to increase the gas pressure by rotating it [28]. They are simple and inexpensive but are only applicable to low compression ratios. Reciprocating compressors use the reciprocating motion of the piston to compress the gas. These compressors have a wide range of applications in the gas processing industry and can operate at high compression ratios.
for lower flow rates. Among all, reciprocating compressor satisfies the requirements (high compression ratio, size, weight, cost) of the proposed system.

In the reciprocating compressor, the rotary motion of the compressor shaft provided by the electric motor is converted to reciprocating motion of the piston by connecting the crankshaft, connecting rod and piston pin to it. The suction and discharge valves are located at the top of the cylinder. Typically, reed valves are used. Figure 5-4 shows the major components of the typical reciprocating compressor, which are identified as Piston, Connecting rod, Crankshaft, Cylinder, Valve plate, Crankcase, and an electric motor.

![Figure 5-4 Parts of compressor](image)

5.2.1 Design

Figure 5-5 shows a P-V diagram of the reciprocating compressor. At state 4, movement of the piston towards the outer dead center creates a vacuum inside the cylinder. The pressure difference between cylinder and suction chamber opens the suction valve which allows gas flow inside the cylinder. Once it reaches the bottom dead center (state 1), the compression begins as the piston moves towards the
top dead center which closes the suction valve. When the cylinder pressure reaches discharge pressure, the discharge valve opens to eject compressed air at state 2. At state 3, the piston reaches top dead center which closes the discharge valve then, the clearance gas expands as it moves towards the bottom dead center.

![Figure 5-5 Thermodynamic compression cycle](image)

The process of the ideal thermodynamic compression cycle is identified as

- Process 4-1: Isobaric gas induction
- Process 1-2: Isentropic compression
- Process 2-3: Isobaric gas delivery
- Process 3-4: Isentropic expansion

The primary step in the design process is to identify the volume at each state of the compression process. This can be achieved by determining the mass of gas per cycle, which is the ratio of the mass flow rate \( m_{dot} \) to rotations per second (rps).
The volume at state 1 is the total volume required for the mass per cycle at suction pressure and temperature, which can be calculated using the ideal gas equation as

\[ V_1 = \frac{R T_s}{P_s} m_{cyc} \] (5.12)

The volume at state 2 is the volume required for the mass per cycle at discharge pressure and temperature which is

\[ V_2 = \frac{R T_d}{P_d} m_{cyc} \] (5.13)

The volume at state 3 is called the clearance volume \( V_c \). Heinz P. Bloch et al., [30] suggested the minimum clearance ratio of a typical reciprocating compressor as 4% to 16%. The proposed system assumes 4.7% and 16% clearance ratio for compressor 1 and 2 to satisfy the design requirements. The clearance volume is calculated as

\[ V_c = V_3 = 0.04 V_1 \text{ or } 0.16 V_1 \] (5.14)

The volume at state 4 is the swept volume \( V_s \) required for the piston, which can be calculated from total volume \( V_1 \) and volume at state 2 \( V_2 \) as

\[ V_s = V_1 - V_2 \] (5.15)

The compression ratio is determined from the swept and clearance volume. This value should be equal to the required compression ratio to validate the clearance ratio assumption

\[ CR = \frac{V_s + V_c}{V_c} \] (5.16)
Once the swept volume is determined, the next step is to calculate the bore and stroke required for the compressor. Stroke (S) to Bore (B) ratio plays a vital role in the design. Dennis N. Assanis et al.,[31] recommended the 1.3 Stroke/Bore ratio from their simulation results. The bore is calculated using the cylindrical geometric relationship as

$$B = \sqrt{\frac{4V_d}{\pi S}}$$  \hspace{1cm} (5.17)

The design parameters of the compressors are shown in Table 5-2.

Table 5-2 Design parameters of the compressors

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Compressor 1</th>
<th>Compressor 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Angular velocity (ω)</td>
<td>3600 RPM (Assumption)</td>
<td>60 RPM (Assumption)</td>
</tr>
<tr>
<td>Mass per cycle (m_{cyc})</td>
<td>6.94 \times 10^{-5} kg</td>
<td>1.11 \times 10^{-3} kg</td>
</tr>
<tr>
<td>Volume at state 1 (V_1)</td>
<td>0.057 L</td>
<td>0.011 L</td>
</tr>
<tr>
<td>Volume at state 2 (V_2)</td>
<td>0.003 L</td>
<td>0.0044 L</td>
</tr>
<tr>
<td>Volume at state 3 (V_c)</td>
<td>0.0026 L</td>
<td>0.0019 L</td>
</tr>
<tr>
<td>Volume at state 4 (V_d)</td>
<td>0.054 L</td>
<td>0.0079 L</td>
</tr>
<tr>
<td>Compression ratio (CR)</td>
<td>21.12 (Satisfied)</td>
<td>5 (Satisfied)</td>
</tr>
<tr>
<td>Bore (B)</td>
<td>37.48 mm</td>
<td>19.06 mm</td>
</tr>
<tr>
<td>Stroke (S)</td>
<td>48.73 mm</td>
<td>24.78 mm</td>
</tr>
</tbody>
</table>

The design methodology of major components (Piston, connecting rod, Crankshaft) is briefly discussed.
5.2.1.1 Piston

The Piston is a reciprocating part of the compressor which compresses the gas by its reciprocating motion. The typical materials used are Cast Iron, Aluminum Alloy, and Cast Steel. Figure 5-6 shows the important parameters required for the piston design.

![Figure 5-6 Piston parameters [32]](image)

The thickness of the piston head \( (t_H) \) is calculated using Grashoff’s formula based on discharge pressure \( (P_d) \) and permissible yield strength of the material \( (\sigma_t) \) as

\[
t_H = B \sqrt{\frac{3 P_d B^2}{16 \sigma_t}}
\]

(5.18)

The piston rings are used to maintain the seal between piston and cylinder bore. There are two types of piston rings such as compression (or pressure rings) and oil rings. The compression ring prevents the fluid leakage to the crankcase whereas, the oil ring prevents oil leakage to the cylinder. Three piston rings are chosen for the proposed design. The radial thickness \( (t_1) \) of a piston is mainly depending on the gas pressure on cylinder walls \( (P_w) \) which are typically assumed as 0.025 MPa to 0.042 MPa.
\[ t_1 = B \frac{3 P_w}{\sigma_t} \quad (5.19) \]

The minimal axial thickness is calculated, based on the number of rings \( n_r \)

\[ t_2 = \frac{B}{10 n_r} \quad (5.20) \]

The width of top land \( b_1 \) from piston head thickness is calculated as

\[ b_1 = 1.2 t_H \quad (5.21) \]

The width of other land \( b_2 \) is determined from the axial thickness as

\[ b_2 = 0.75 t_2 \quad (5.22) \]

The piston barrel is a cylindrical portion of the piston. The minimum piston barrel thickness at an open end \( t_3 \) determined from the relation [32].

\[ t_3 = 0.03 B + t_H \quad (5.23) \]

The minimum piston barrel thickness \( t_4 \) at the open end is

\[ t_4 = 0.35 t_3 \quad (5.24) \]

The section of the piston under the grooves is called as piston skirt, length of the piston skirt \( L_s \) is

\[ L_s = 0.65 B \quad (5.25) \]

The total length of the piston \( L \) is

\[ L = L_s + 2 b_2 + 3 t_2 + b_1 \quad (5.26) \]
Once the important design parameters of the piston are determined, the next step is to design piston pin or gudgeon pin. It is a hollow cylinder (tapered inside), which is used to connect the piston to connecting rod. The piston pin is to be designed for maximum load exerted by compressed gas which is

\[ F_g = \frac{\pi}{4} B^2 P_d \]  \hspace{1cm} (5.27)

The load due to bearing pressure is

\[ F_b = P_b d_o l_1 \]  \hspace{1cm} (5.28)

The outside diameter \( d_o \) of the pin is determined by equating the load due to bearing pressure and the load due to maximum gas pressure as

\[ d_o = \frac{F_g}{P_b l_1} \]  \hspace{1cm} (5.29)

The inside diameter of the pin \( d_i \) from the outside diameter is

\[ d_i = 0.6 d_o \]  \hspace{1cm} (5.30)

The center of the piston pin should be from 0.02 B to 0.04 B above the center of the skirt. The length of the piston pin \( l_1 \) in the connecting rod bush is taken as 0.45 B.

The inputs required for the piston 1 and piston 2 design are tabulated in Table 5-3.

<table>
<thead>
<tr>
<th>Input parameter</th>
<th>Piston 1</th>
<th>Piston 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>Aluminum alloy</td>
<td>Steel alloy</td>
</tr>
<tr>
<td>Parameter</td>
<td>Piston 1</td>
<td>Piston 2</td>
</tr>
<tr>
<td>---------------------------------</td>
<td>----------</td>
<td>----------</td>
</tr>
<tr>
<td>Factor of safety</td>
<td>2.25</td>
<td>2.25</td>
</tr>
<tr>
<td>Tensile yield strength</td>
<td>275 MPa</td>
<td>620 MPa</td>
</tr>
<tr>
<td>Gas pressure on cylinder wall</td>
<td>0.042 MPa (Assumption)</td>
<td>0.042 MPa (Assumption)</td>
</tr>
<tr>
<td>Bearing material</td>
<td>Bronze</td>
<td>Steel</td>
</tr>
<tr>
<td>Allowing Bearing pressure</td>
<td>50 MPa</td>
<td>100 MPa</td>
</tr>
</tbody>
</table>

The final design dimensions of the pistons are obtained and are tabulated in Table 5-4.

Table 5-4 Final dimensions for the piston design

<table>
<thead>
<tr>
<th>Final design Parameter</th>
<th>Piston 1</th>
<th>Piston 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Piston head thickness (t_{H})</td>
<td>3.49 mm</td>
<td>2.33 mm</td>
</tr>
<tr>
<td>Radial thickness (t_1)</td>
<td>1.2 mm</td>
<td>0.40 mm</td>
</tr>
<tr>
<td>Number of rings</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Axial thickness (t_2)</td>
<td>1.25 mm</td>
<td>0.63 mm</td>
</tr>
<tr>
<td>Width of the top land (b_1)</td>
<td>4.19 mm</td>
<td>2.80 mm</td>
</tr>
<tr>
<td>Width of other ring lands (b_2)</td>
<td>0.937 mm</td>
<td>0.47 mm</td>
</tr>
<tr>
<td>Top end piston barrel thickness (t_3)</td>
<td>4.616 mm</td>
<td>2.90 mm</td>
</tr>
<tr>
<td>Open end piston barrel thickness (t_4)</td>
<td>1.616 mm</td>
<td>1.01 mm</td>
</tr>
<tr>
<td>Piston skirt length (L_s)</td>
<td>24.368 mm</td>
<td>12.39 mm</td>
</tr>
<tr>
<td>Total length of the piston (L_p)</td>
<td>34.181 mm</td>
<td>18.056 mm</td>
</tr>
<tr>
<td>Outside diameter of the piston pin (d_o)</td>
<td>7.39 mm</td>
<td>7.342 mm</td>
</tr>
<tr>
<td>Inside diameter of the piston pin (d_i)</td>
<td>4.43 mm</td>
<td>4.40 mm</td>
</tr>
<tr>
<td>Length of the piston pin in the bush (l_1)</td>
<td>16.87 mm</td>
<td>8.58 mm</td>
</tr>
<tr>
<td>Weight (kg)</td>
<td>0.046</td>
<td>0.015</td>
</tr>
</tbody>
</table>

CAD modelling of piston 1 and 2 in shown in figure 5-7 and 5-8.
Figure 5-7 Piston-1 2D and 3D models.

Figure 5-8 Piston-2 2D and 3D models.
5.2.1.2 Connecting rod

The connecting rod connects the piston to the crankshaft by piston pin (or gudgeon pin) and crank pin. This transmits the rotary motion of crankshaft to reciprocating motion of a piston. It is a long shank connected between a small end to the big end. The typical cross-section used in the reciprocating compressor is the I-section. Figure 5-9 shows the cross-section of the connecting rod.

![Figure 5-9 Cross-section of a connecting rod [32]](image)

The alternating direct compressive and tensile forces act on the connecting rod. Leela Krishna et al., [33] identified that the connecting rod should be four times stronger in buckling about y-axis than about x-axis, as the compressive force dominates tensile force. The I-section chosen for the design is as follows.

The thickness of the web and flange section is ‘t’

- Width (B) of the section
  \[ B = 4 \ t \]
- Height (H) of the section
  \[ H = 5 \ t \]
- Area of the cross-section
  \[ A = 11 \ t^2 \]
- Moment of inertia of the section about X-axis
  \[ I_{xx} = \frac{419}{12} \ t^4 \]
Moment of inertia of the section about Y-axis

\[ I_{yy} = \frac{131}{12} t^4 \]

The ratio of x-moment of inertia to y-moment of inertia is 3.2, which is less than suggested moment ratio 4. So, the cross-section selection is valid.

The length of connecting rod \((L_c)\) is calculated from stroke \((S)\) as

\[ L_c = 2S \quad (5.31) \]

The connecting road is to be designed to withstand the maximum buckling load caused by discharge pressure. Which is calculated from discharge pressure with a safety factor \((FS)\),

\[ W_B = \frac{\pi B^2 P_d}{4} FS \quad (5.32) \]

The buckling load can also be expressed using Rankin’s formula,

\[ W_B = \frac{\sigma_c A}{1 + a \left( \frac{L_c}{k_{xx}} \right)^2} \quad (5.33) \]

Where,

\( \sigma_c \) is compressive yield strength.

\( A \) is cross-section area of the section which is 11 t².

\( L_c \) is the length of the connecting rod.

‘a’ is material constant which can be expressed by compressive yield strength and Young’s modulus \((E)\) as \( \frac{\sigma_c}{\pi^2 E} \).

\( k_{xx} \) is the radius of gyration expressed from x-moment of inertia and area of section as \( \sqrt{\frac{I_{xx}}{A}} \).
The thickness of the section is determined by equating above buckling load equations based on which the other dimensions are calculated. The height of the shank at the small and big end is 0.85 and 1.2 respectively. The inner diameter of the small end should be equal to the outer diameter of the piston pin. The outer diameter of the small end is the sum of inner diameter, bush thickness, and marginal thickness.

The inner diameter of the big end is calculated from crank pin geometry. Crank pin connects the connecting rod to the crankshaft. The design of crank pin is explained later. The inputs required for the connecting rod design are tabulated in Table 5-5.

Table 5-5 Input parameters required for connecting rod design

<table>
<thead>
<tr>
<th>Input parameters</th>
<th>Connecting rod 1</th>
<th>Connecting rod 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>Aluminum alloy</td>
<td>Steel alloy</td>
</tr>
<tr>
<td>Compressive yield strength ($\sigma_c$)</td>
<td>275 MPa</td>
<td>723 MPa</td>
</tr>
<tr>
<td>Safety factor (SF)</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Modulus of Elasticity (E)</td>
<td>65 GPa</td>
<td>210 GPa</td>
</tr>
<tr>
<td>Bush material</td>
<td>Bronze</td>
<td>Steel</td>
</tr>
<tr>
<td>Allowable bearing pressure</td>
<td>12.5 MPa</td>
<td>25 MPa</td>
</tr>
<tr>
<td>Marginal thickness</td>
<td>2 mm</td>
<td>2 mm</td>
</tr>
</tbody>
</table>

The final design parameters of the connecting rod are tabulated in Table 5-6.

Table 5-6 Final design parameters of connecting rods

<table>
<thead>
<tr>
<th>Final design parameters</th>
<th>Connecting rod 1</th>
<th>Connecting rod 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length of the connecting rod (L)</td>
<td>97.47 mm</td>
<td>49.57 mm</td>
</tr>
<tr>
<td>Thickness of the section (t)</td>
<td>3.68 mm</td>
<td>2.23 mm</td>
</tr>
<tr>
<td>Height of the section at big end (H_1)</td>
<td>22.08 mm</td>
<td>13.42 mm</td>
</tr>
<tr>
<td>Height of the section at small end (H_2)</td>
<td>15.64 mm</td>
<td>9.511 mm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------------------------</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>Inner diameter of the small end ($d_{si}$)</td>
<td>7.39 mm</td>
<td>7.34 mm</td>
</tr>
<tr>
<td>Outer diameter of the small end ($d_{so}$)</td>
<td>15.39 mm</td>
<td>9.34 mm</td>
</tr>
<tr>
<td>Inner diameter of the big end ($d_{bi}$)</td>
<td>19.59 mm</td>
<td>13.92 mm</td>
</tr>
<tr>
<td>Outer diameter of the big end ($d_{bo}$)</td>
<td>29.60 mm</td>
<td>15.99 mm</td>
</tr>
<tr>
<td>Weight (kg)</td>
<td>0.062</td>
<td>0.022</td>
</tr>
</tbody>
</table>

CAD modelling of connecting rods 1 and 2 shown in figure 5-10

![Figure 5-10 2D and 3D models of the connecting rod 1 and 2](image)

5.2.1.3 Crankshaft

Crankshaft converts the rotary motion of an electric motor to reciprocating motion of the piston, by means of connecting rod. It comprises shafts, bearings, crank webs (or arms), and crankpin. There are two types of crankshaft geometries based on the crank pin position. When crankpin is in the center it is called Centre Crankshaft and as Side crankshaft, if it’s at the side. The Centre Crankshaft geometry
is used in the proposed design for its stability and proved utilization in small reciprocating compressors.

There are two forces acting on the crankshaft depends on crank position. When the crank is at dead center, piston transmits the maximum force on to crankpin which causes maximum bending stress on the crankshaft. When the crank is at an angle, the twisting stress dominates bending stress. The crankshaft design is based on either condition of the crank. The proposed crankshaft is designed at the crank which is at dead center. Figure 5-11 shows typical crankshaft and forces associated with it.

![Crankshaft diagram](image)

Figure 5-11 crankshaft

The maximum load on piston due to discharged gas pressure is calculated from equation 5.27. When piston load acts on a crank pin in the normal direction, it exerts two horizontal reaction forces on shaft 1 and 2. The load is assumed to be distributed equally along the shaft. The reaction forces can be expressed by the maximum gas load ($F_g$) and the distance between shaft centers ($b$).

\[
H_1 = \frac{F_g b_1}{b} \quad H_2 = \frac{F_g b_2}{b}
\]

(5.34)
The crankpin is designed by assuming maximum bending moment at the center of pin, which can be determined by horizontal reaction force ($H_1$) as,

$$M_c = H_1 b_2$$  \hspace{1cm} (5.35)

The bending moment can also be calculated from maximum allowable bending stress ($\sigma_b$),

$$M_c = \frac{\pi}{32} (d_c)^3 \sigma_b$$  \hspace{1cm} (5.36)

The required crank diameter is determined by equating (5.35) & (5.36) equations. The crank pin length is obtained by assuming allowable bearing pressure ($P_b$) as

$$l_c = \frac{F_g}{d_c P_b}$$  \hspace{1cm} (5.37)

Crank web thickness ($t$) and crank web width ($w$), are calculated using the empirical relations based on bore diameter ($B$) and crank pin diameter ($d_c$),

$$t = 0.32 B$$
$$W = 1.12 d_c + 12.7 \text{ mm}$$  \hspace{1cm} (5.38)

The required shaft diameter is calculated using the relation based on crank web thickness ($t$),

$$d_s = \frac{t}{0.6}$$  \hspace{1cm} (5.39)

The final dimensions of the crankshafts are tabulated below in Table 5-7.
Table 5-7 Final design of crankshafts

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Crankshaft 1</th>
<th>Crankshaft 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crank pin diameter ($d_c$)</td>
<td>19.59 mm</td>
<td>13.92 mm</td>
</tr>
<tr>
<td>Length of the crank pin ($L$)</td>
<td>25.47 mm</td>
<td>18.09 mm</td>
</tr>
<tr>
<td>Thickness of the crank web ($t$)</td>
<td>11.99 mm</td>
<td>6.1 mm</td>
</tr>
<tr>
<td>Width of the crank web ($W$)</td>
<td>22.04 mm</td>
<td>15.66 mm</td>
</tr>
<tr>
<td>Diameter of the shaft ($d_s$)</td>
<td>19.99 mm</td>
<td>10.16 mm</td>
</tr>
<tr>
<td>Weight (kg)</td>
<td>0.145</td>
<td>0.098</td>
</tr>
</tbody>
</table>

CAD modeling of crankshaft 1 and 2 are shown in Figure 5-12.

Figure 5-12 2D and 3D models of the crankshaft 1 and 2
5.2.2 FEA structural analysis

The Structural integrity of the design is validated using FEA Structural analysis of the major parts of the compressor assembly.

CAD modeling of compressor 1 and 2 assemblies.

![Figure 5-13 Compressor 1 and 2 assemblies](image)

The Solidworks simulation is used for the analysis. The initial step in the simulation is to assign material to the components. The next step is to define connecting rod connection in crankpin and piston pin. Later, the assembly is fixed at the shaft position. Once the material, connections and fixture geometry is assigned, the next step is to apply maximum compressor pressure on piston surface.

![Figure 5-14 Meshing and boundary conditions (pressures and fixtures applied) assemblies](image)
The design is validated by obtaining the von Mises stress and Factor of safety of the assembly. It can be observed from Figure 5-15 & 5-16, the von Mises stress is lower than the yield strength of materials and the factor of safety is observed to be 3.7 and 2 for compressor 1 and 2 respectively. Hence, the design is valid.

Figure 5-15 Von-Misses stresses of compressor assembly

Figure 5-16 Factor of safety for compressor 1 and 2
The other parts of the compressor not included in the design due to time constraint are crankcase, valves and an electric motor. The crankcase is responsible to provide lubrication by holding all the components together. There are two types of lubrication systems available in typical reciprocating compressors such as Cylinder lubrication and Crankcase lubrication. The Cylinder lubrication provides lubrication to the piston, piston rings, cylinder liners, cylinder packing, and valve. Whereas, Crankcase lubrication provides lubrication to main bearings, crank pins, piston pins, and crosshead bearing [34]. The lubricated compressor requires both the cylinder and crankcase lubrication system. But, non-lubricated compressor requires only crankcase lubrication which is suggested to use in the proposed system to eliminate oil leakage to compression chamber and valve chambers. Figure 5-17 shows the assembly of compressor 1 and 2 including crankcase (designed based on major parts).

![Figure 5-17 Final assemblies of compressors 1 and 2](image)

Compressor valves are the devices placed above the cylinder which regulates the cycle of operations in a cylinder. These valves act as a check valve (one-way valve) which solely opened by the pressure difference across the valve. The selection of the compressor valves depends on the Valve seat geometry, sealing element and the nature of damping used to control the motion. The typical valves based on valve seat geometry are Rectangular valves, Concentric ring valves, Ported Plate valves, and Disc (Poppet) valves. The Rectangular valves are further divided into feather valves, channel valves, and reed valves. The reed valve is recommended to be the best fit the proposed system for its operational capabilities of high-pressure applications and ease of operation. Figure 5-18 shows typical reed valve geometry.
Figure 5-18 Typical reed valve geometry

The electric motor provides the rotary motion to the crankshaft. The drone motors are the perfect fit for the proposed compressors because these are very compact and powerful. The operation of these motors is different from the typical motors used in the compressor, the case surrounding the motor rotates and the inside of the motor is stationary. Brushless out runner DC electric motors are suggested to use in the compressors. The specifications of the electric motors are shown below:

Table 5-8 Specifications of commercial electric motor.

<table>
<thead>
<tr>
<th>Specifications</th>
<th>Electric motor 1</th>
<th>Electric motor 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer</td>
<td>E-flite (Horizon Hobby)</td>
<td>E-flite (Horizon Hobby)</td>
</tr>
<tr>
<td>Power</td>
<td>Up to 6000 watts</td>
<td>Up to 275 watts</td>
</tr>
<tr>
<td>Cells</td>
<td>12S Li-Po</td>
<td>3S Li-Po</td>
</tr>
<tr>
<td>Shaft diameter</td>
<td>10 mm</td>
<td>4 mm</td>
</tr>
<tr>
<td>Weight</td>
<td>1.240 kg</td>
<td>0.087 kg</td>
</tr>
</tbody>
</table>

The total weight of the compressor 1 and 2 are estimated from the design (including crankcase, valves and electric motor) are 3.5 kg and 2 kg respectively.
5.3 Heat exchanger design and conjugate heat transfer analysis

The objective of this section is to design heat exchangers to cool the biogas from 908.68 K to liquefaction temperature (216 K). As discussed in process design section, the proposed system requires two heat exchangers to achieve the required heat dissipation. The design requirements of heat exchangers are shown in table 5-9.

Table 5-9 design requirements of heat exchangers

<table>
<thead>
<tr>
<th>Design requirements</th>
<th>Heat exchanger 1</th>
<th>Heat exchanger 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet temperature</td>
<td>908.68 K</td>
<td>374.33 K</td>
</tr>
<tr>
<td>Required outlet temperature</td>
<td>374.33 K</td>
<td>206.38 K</td>
</tr>
<tr>
<td>Required heat dissipation</td>
<td>3.42 kW</td>
<td>0.822 W</td>
</tr>
</tbody>
</table>

The key constraints for the heat exchanger design are weight, size, cost, and the convective fluid. Figure 5-19 shows the broad classification of heat exchangers based on their construction. The typical heat exchangers used in the gas processing industry are Double pipe heat exchanger, Shell and tube heat exchanger, Plate and frame heat exchangers, tube-fin heat exchangers, Spiral heat exchangers, etc. Among all, forced convective tube-fin heat exchanger is chosen for its Proven cooling abilities of pressurized gases and freedom to select convective fluid [35].

![Classification of heat exchangers based on their construction](image-url)
5.3.1 The optimum design of tube-fin heat exchanger

In the tube-fin heat exchanger, the hot fluid flows inside the tube and the convective or cold fluid flows across the tube to dissipate heat from hot fluid to cold fluid. The heat dissipation is increased by either increasing thermal conductivity or total heat transfer area of the fins or by increasing the heat transfer coefficient of convective fluid. Figure 5-20 shows terminology of tube-fin heat exchanger used in the design where ‘t’ is thickness of the fin, ‘z’ is fin spacing, ‘w’ is length of the pipe, ‘r₁’ is inner diameter of the tube, ‘a’ is fin width, ‘T₀’ is coolant temperature, and ‘U₀’ is convective fluid velocity.

![Figure 5-20 Tube-fin heat exchanger](image)

The initial step is, to find the properties of each fluid at film temperature (average of initial inlet and desired outlet temperature). The required heat dissipation is calculated using the first law of thermodynamics neglecting kinetic, potential and network done on the system.

\[ Q_{dis} = m \dot{c}_p \Delta T \] (5.40)

Later, a suitable tube is found to meet the design pressure and temperature with the factor of safety. This is completed using the Boardman formula (ASTM B210) as a function of outer tube diameter (D₀), thickness (t) and yield strength (σ_yield) of the material.
\[
\sigma_{allow} = \frac{2 \sigma_{yield} t}{D_0 SF - 0.8 t}
\] (5.41)

The optimum tube-fin design equations proposed by Dr. Lee (Wiley, 2011) are,

The Reynolds number as a function of fin width \((a)\), convective fluid velocity \((U_\infty)\) and kinematic viscosity \((\nu)\)

\[
Re = \frac{U_\infty a}{\nu}
\] (5.42)

The optimum fin spacing as a function of Convective Reynolds number \((Re)\) and Prandtl number \((Pr)\)

\[
z_{opt} = a \ 3.24 \ Re^{-\frac{1}{2}} \ Pr^{-\frac{1}{4}}
\] (5.43)

The average Heat transfer coefficient as a function of thermal conductivity \((k)\), Reynolds number \((Re)\) and Prandtl number \((Pr)\)

\[
h = \frac{k}{a} \ 0.664 \ Re^{\frac{1}{2}} \ Pr^{-\frac{1}{4}}
\] (5.44)

The fin efficiency is calculated from the Bessel’s relation as

\[
\eta_f = C_1 \frac{K_1(mr_1)K_1(mr_2) - I_1(mr_1)I_1(mr_2)}{I_0(mr_1)K_1(mr_2) + K_0(mr_1)I_1(mr_2)}
\] (5.45)

Where, \(C_1 = \frac{2 r_1/m}{r_2^2 - r_1^2}\), \(m = \left(\frac{2h}{kt}\right)^\frac{1}{2}\), \(r_1 = \frac{d}{2}\), \(r_2 = \frac{a}{\pi}\).

The total number of fins as a function of pipe length \((W)\), optimum spacing \((z)\) and thickness \((t)\)
\[ n_f = \frac{W}{z + t} \] (5.46)

The single fin area \((A_f)\) is determined by radii and thickness as

\[ A_f = 2\pi (r_2^2 - r_1^2) + 2\pi r_2 t \] (5.47)

The total heat transfer area \((A_t)\) is

\[ A_t = n_f (A_f + 2\pi r_1 z_{opt}) \] (5.48)

The overall surface efficiency \((\eta_o)\) is obtained as

\[ \eta_o = 1 - n_f \frac{A_f}{A_t} (1 - \eta_f) \] (5.49)

The outlet temperature \((T_0)\) is

\[ T_0 = \frac{Q_{dis}}{\eta_o h A} + T_{inf} \] (5.50)

Length of the pipe \((W_{req})\) required

\[ W_{req} = (z_{opt} + t) n_f \] (5.51)

Mass of the pipe \((m_p)\) required

\[ m_p = \rho_{pipe} \pi W \left( \left( \frac{D_o}{2} \right)^2 - r_1^2 \right) \] (5.52)

Mass of the fin \((m_f)\)

\[ m_f = \rho_{pipe} \pi t (r_1^2 - r_1^2) n_f \] (5.53)

Total mass of the heat exchanger \((m_{he})\)
\[ m_{he} = m_p + m_f \] (5.54)

The biogas pressure drop is calculated using,

\[ \Delta P = 2 f \left( \frac{W}{d_i} \right) (\rho_{bio} V_{bio}^2) \] (5.55)

Where \( f \) is the fanning friction factor taken as 0.2 from the moody chart based on biogas Reynolds number.

\( V_{bio} \) is the velocity of biogas inside the pipe which is calculated by

\[ V_{bio} = \frac{m_{dot}}{\rho_{bio} \pi d_i^2} \]

The Reynolds number of biogas flowing inside the pipe is

\[ Re_{bio} = \frac{4 m_{dot}}{\pi d_i \mu} \]

An iterative Mathcad program is developed using the optimum tube – fin design equations as a function of thickness (t), Pipe length (W), Fin width (a) and coolant velocity \( (U_\infty) \). Figure 5-21 shows the process flow of the optimal tube – fin design Mathcad program.

Figure 5-21 Process flow of the optimal tube – fin design
Standard 1/8” schedule 10 bare aluminum 6061 – T6 pipe satisfies the design requirements with safety factor 3. The properties of biogas at film temperatures of heat exchanger 1 and 2 are shown below in Table 5-10.

Table 5-10 Properties of biogas at film temperatures

<table>
<thead>
<tr>
<th>Property</th>
<th>Biogas (641.50 K)</th>
<th>Biogas (290.89 K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific heat at constant pressure (C_p)</td>
<td>1.53 kJ/kg K</td>
<td>1.16 kJ/kg K</td>
</tr>
<tr>
<td>Dynamic viscosity (μ)</td>
<td>2.72 × 10^{-5} kg/m s</td>
<td>1.40 × 10^{-5} kg/m s</td>
</tr>
<tr>
<td>Kinematic viscosity (ν)</td>
<td>8.54 × 10^{-7} m^2/s</td>
<td>4.41 × 10^{-7} m^2/s</td>
</tr>
<tr>
<td>Thermal conductivity (k)</td>
<td>0.043 W/m K</td>
<td>0.021 W/m K</td>
</tr>
<tr>
<td>Density (ρ)</td>
<td>31.48 kg/m^3</td>
<td>54.41 kg/m^3</td>
</tr>
</tbody>
</table>

As discussed in section 5.1.2., the ambient air is used as a convective fluid for heat exchanger 1 whereas, expanded liquid CO_2 is used for heat exchanger 2. The properties of convective fluids at inlet temperature are shown below in Table 5-11.

Table 5-11 Properties of convective fluids at inlet temperatures

<table>
<thead>
<tr>
<th>Property</th>
<th>Ambient air (300 K)</th>
<th>Expanded CO_2 (156.91 K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific heat at constant pressure (C_p)</td>
<td>1.00 kJ/kg K</td>
<td>0.838 kJ/kg K</td>
</tr>
<tr>
<td>Dynamic viscosity (μ)</td>
<td>1.84 × 10^{-5} kg/m s</td>
<td>1.45 × 10^{-5} kg/m s</td>
</tr>
<tr>
<td>Kinematic viscosity (ν)</td>
<td>1.56 × 10^{-5} m^2/s</td>
<td>7.88 × 10^{-6} m^2/s</td>
</tr>
</tbody>
</table>
Thermal conductivity (k) | $0.026 \frac{W}{m \, K}$ | $0.034 \frac{W}{m \, K}$
---|---|---
Density ($\rho$) | $1.17 \frac{kg}{m^3}$ | $1.84 \frac{kg}{m^3}$

After numerous iterations, the final input properties of heat exchangers are shown in Table 5-12.

Table 5-12 Final input properties of heat exchangers

<table>
<thead>
<tr>
<th>Property</th>
<th>Heat exchanger 1</th>
<th>Heat exchanger 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fin thickness (t)</td>
<td>1.2 mm</td>
<td>1.2 mm</td>
</tr>
<tr>
<td>Pipe length (W)</td>
<td>1.5 mm</td>
<td>1.2 mm</td>
</tr>
<tr>
<td>Fin width (a)</td>
<td>40 mm</td>
<td>40 mm</td>
</tr>
<tr>
<td>Convective fluid velocity ($U_{\infty}$)</td>
<td>9.55 m/s</td>
<td>1.72 m/s</td>
</tr>
</tbody>
</table>

The final output properties of the heat exchangers are tabulated in Table 5-13.

Table 5-13 Output properties of the heat exchangers

<table>
<thead>
<tr>
<th>Property</th>
<th>Heat exchanger 1</th>
<th>Heat exchanger 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet temperature ($T_0$)</td>
<td>375.41 K</td>
<td>207.33 K</td>
</tr>
<tr>
<td>Optimum fin spacing ($z_{opt}$)</td>
<td>0.904 mm</td>
<td>1.792 mm</td>
</tr>
<tr>
<td>Average heat transfer coefficient of Convective fluid ($h$)</td>
<td>60.15 W/m^2*K</td>
<td>37.475 W/m^2*K</td>
</tr>
<tr>
<td>Average heat transfer coefficient of biogas ($h_{bio}$)</td>
<td>4.82 W/m^2*K</td>
<td>6.03 W/m^2*K</td>
</tr>
<tr>
<td>Number of radial fins ($n_f$)</td>
<td>713</td>
<td>402</td>
</tr>
<tr>
<td>Total heat transfer area ($A_t$)</td>
<td>0.791 m^2</td>
<td>0.448 m^2</td>
</tr>
<tr>
<td>Overall surface efficiency ($\eta_o$)</td>
<td>95 %</td>
<td>97 %</td>
</tr>
<tr>
<td>Mass of heat exchanger ($m_{he}$)</td>
<td>1.204 kg</td>
<td>0.688 kg</td>
</tr>
</tbody>
</table>
Pressure drop ($\Delta P$) | 2.69 bar | 2.15 bar

From the table, it can be observed that the ambient air velocity is not enough to achieve the required heat dissipation of heat exchanger 1. So, forced convection is needed to provide the required air velocity. Forced convection is achieved by attaching a fan to heat exchanger. A commercial round axial fan of 10” inch (254 mm) diameter is chosen for its high volumetric flow capacity (500 CFM). The pipe is turned 180 degrees to provide constant air velocity throughout the effective heat transfer area. The heat exchanger 1 is enclosed in a box (250 × 240 × 40 mm), this constraint makes the 1.5 m single pipe to 6 pipes of dimension 250 mm each. These pipes are joined by pipe bends of radius 40 mm (which is the fin width). Heat exchanger 2 uses liquid CO$_2$ as a convective fluid by expanding it from liquefaction pressure to ambient pressure (0.101 MPa). This expansion requires an expansion valve to control the velocity of the expanded CO$_2$ gas. The box (240 × 200 × 40 mm) is chosen based on heat exchanger 2 dimensions. The final dimensions of the heat exchangers are shown below in Table 5-14.

Table 5-14 Final dimensions of the heat exchangers

<table>
<thead>
<tr>
<th>Final design</th>
<th>Heat exchangers 1</th>
<th>Heat exchanger 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size (W × H × D)</td>
<td>250 × 240 × 40</td>
<td>240 × 200 × 40</td>
</tr>
<tr>
<td>Inside diameter of the pipe</td>
<td>2.98 mm</td>
<td>2.98 mm</td>
</tr>
<tr>
<td>Outside diameter of the pipe</td>
<td>4.76 mm</td>
<td>4.76 mm</td>
</tr>
<tr>
<td>Number of rectangular fins</td>
<td>119</td>
<td>81</td>
</tr>
<tr>
<td>Fin spacing</td>
<td>0.904</td>
<td>1.792 mm</td>
</tr>
<tr>
<td>Fin thickness</td>
<td>1.2 mm</td>
<td>1.2 mm</td>
</tr>
<tr>
<td>Mass</td>
<td>1.204</td>
<td>0.688 kg</td>
</tr>
<tr>
<td>Mass of fan</td>
<td>0.500 kg</td>
<td>...........</td>
</tr>
</tbody>
</table>

CAD modeling of heat exchanger 1 and 2 shown in Figure 5-22.
5.3.2 CFD Conjugate heat transfer analysis

Conjugate heat transfer analysis is performed to verify the heat exchanger design using ANSYS - CFX. The analysis involves the following steps.

Step 1- Import Geometry to ANSYS design modular.

The imported geometry is shown in Figure 5-23.

![Figure 5-23 3D models of heat exchanger 1 and 2](image)

- a) Heat exchanger body.
- b) Biogas body.
c) Convective fluid body. 

Figure 5-23 Heat exchanger geometry

Step 2 - Meshing in ANSYS - Mesh

Meshing plays an important role in accurately solving the model as all the governing equations are solved in discretized nodes. ANSYS Default mesh is used in the present analysis.
Figure 5-24 Heat exchanger meshing

Figure 5-24 (b) Highlights the named selections of the mesh, where A, B, C represents the domains of convective fluid (this case air), heat exchanger and biogas respectively. D, E, F, G represents the boundaries of biogas in, biogas out, convective fluid in and convective fluid out.

Step 3- Problem Setup in ANSYS – CFX (pre)

In Figure 5-25 (a), the arrow symbols denote the boundary conditions of the domains. b) shows the problem setup tree, where symbol denotes the domain type and symbol donates the boundary conditions.

(a) HE surrounded by convective fluid.  

(b) Problem setup tree Figure.  

Figure 5-25 Problem setup
The problem setup in steady state conjugate heat transfer analysis is divided into three parts such as

1. Domain type and model setup is completed by assigning the material and the model for each domain as shown in Table 5-15.

<table>
<thead>
<tr>
<th>Input</th>
<th>Biogas domain</th>
<th>Air domain</th>
<th>CO₂ domain</th>
<th>He domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain type</td>
<td>Fluid</td>
<td>Fluid</td>
<td>Fluid</td>
<td>Solid</td>
</tr>
<tr>
<td>Material</td>
<td>Biogas</td>
<td>Air ideal gas</td>
<td>Carbon dioxide</td>
<td>Aluminum</td>
</tr>
<tr>
<td>Morphology</td>
<td>Continuous fluid</td>
<td>Continuous fluid</td>
<td>Continuous fluid</td>
<td>Continuous solid</td>
</tr>
<tr>
<td>Reference pressure</td>
<td>Critical pressure</td>
<td>1 bar</td>
<td>1 bar</td>
<td>-----------</td>
</tr>
<tr>
<td>Heat transfer model</td>
<td>Thermal energy</td>
<td>Thermal energy</td>
<td>Thermal energy</td>
<td>Thermal energy</td>
</tr>
<tr>
<td>Turbulence model</td>
<td>k-Epsilon</td>
<td>k-Epsilon</td>
<td>k-Epsilon</td>
<td>-----------</td>
</tr>
<tr>
<td>Heat flux</td>
<td>--------------</td>
<td>------------</td>
<td>------------</td>
<td>-----------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4.3 kW/m² (He 1)</td>
<td>1.8 kW/m² (He 2)</td>
</tr>
</tbody>
</table>

2. Boundary conditions are defined for each fluid domain as shown in Table 5-16.

<table>
<thead>
<tr>
<th>Input</th>
<th>Biogas in</th>
<th>Biogas out</th>
<th>Air in</th>
<th>Air out</th>
<th>CO₂ in</th>
<th>CO₂ out</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow regime</td>
<td>Subsonic</td>
<td>Subsonic</td>
<td>Subsonic</td>
<td>Subsonic</td>
<td>Subsonic</td>
<td>Subsonic</td>
</tr>
<tr>
<td>Normal fluid velocity in</td>
<td>--------------</td>
<td>--------------</td>
<td>9.55 m/s</td>
<td>1.77 m/s</td>
<td>--------------</td>
<td>--------------</td>
</tr>
<tr>
<td>Mass flow rate in</td>
<td>15 kg/hr</td>
<td>--------------</td>
<td>--------------</td>
<td>--------------</td>
<td>--------------</td>
<td>--------------</td>
</tr>
<tr>
<td>Inlet temperature of He1</td>
<td>908.68 K</td>
<td>300 K</td>
<td>--------------</td>
<td>--------------</td>
<td>--------------</td>
<td>--------------</td>
</tr>
<tr>
<td>Inlet temperature of He2</td>
<td>375.414 K</td>
<td>--------------</td>
<td>--------------</td>
<td>156.91 K</td>
<td>--------------</td>
<td>--------------</td>
</tr>
<tr>
<td>Outlet relative pressure</td>
<td>--------------</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
3. Fluid solid interface is defined as shown in Table 5-17.

Table 5-17 Fluid solid interface

<table>
<thead>
<tr>
<th>Input at interface</th>
<th>Biogas to He 1</th>
<th>Biogas to He 2</th>
<th>Air to He 1</th>
<th>CO₂ to He 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average heat – transfer</td>
<td>4.82 W/m²*K</td>
<td>6.03 W/m²*K</td>
<td>60.15 W/m²*K</td>
<td>37.47 W/m²*K</td>
</tr>
<tr>
<td>Coefficient</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Average fluid temperature</td>
<td>641.50 K</td>
<td>290.89 K</td>
<td>320 K</td>
<td>180 K</td>
</tr>
</tbody>
</table>

Step 4 - Numerical solution in CFX-solver manager

An iterative solution is obtained by solving mass, moment, energy and turbulent equations for both the fluids using the finite volume method. The solution converges at around 220 iterations which took about 9 hours to complete the solution. Figure 5-26 (a) shows the convergence of mass and momentum equations of convective fluid, it can be stated that similar convergence is achieved for the rest of the equations.

Figure 5-26 Convergence criteria and workflow
Step 5 - Results in CFD - Post-processing

Figure 5-27 & 5-28 shows the contours of biogas temperature in HE1 and HE2, it can be observed that the average outlet temperatures of HE1 and HE2 are 383.5 K, 195.5 K respectively.
Figure 5-29 & 5-30 depicts the temperature contours of convective fluid at fluid outlet. The maximum temperature is observed at biogas inlet location which is 329 K for convective fluid 1 and 171 K for convective fluid 2.

Figure 5-29 Temperature contours of convective fluid 1 (air) at the outlet

Figure 5-30 Contours of convective fluid 2 (expanded liquid CO₂) temperature at the outlet
Figure 5-31 & 5-32 shows the velocity vectors of convective fluid 1 and convective fluid 2. The maximum velocity is observed at the fin spacing which is 38 m/s for convective fluid 1 and 13 m/s for convective fluid 2.

![Figure 5-31 Velocity vectors of convective fluid 1](image1)

![Figure 5-32 Velocity vectors of convective fluid 2](image2)
Table 5-18 compares the ANSYS - CFX simulation results with Mathcad design. It can be seen that the ANSYS – CFX simulations successfully validate the Mathcad design with less than 5 % error. Hence, the design is valid.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet biogas temperature</td>
<td>375.41 K</td>
<td>383.5 K</td>
<td>207. 33 K</td>
<td>195.5 K</td>
</tr>
</tbody>
</table>

5.4 Liquid-Gas separator design and multi-phase analysis

Based on biogas phase diagram (shown in figure 3-6), CO$_2$ is expected to transform phase from gas to liquid at heat exchanger 2 outlet. This two-phase mixture is sent to phase separator typically called Liquid Gas Separator (LGS). The goal of LGS is to separate the dispersed fluid (CO$_2$ liquid) from continuous fluid (CH$_4$ gas). The separator selection is mainly based on flow regime, separation methodology, and separator geometry. The flow regime depends on the interface between continuous and dispersed fluids. The typical flow regimes are Droplet flow, Plug flow, Stratified flow, Wavy flow, Slug flow, and Annular flow. The inlet flow is assumed to be the droplet flow, as the CO$_2$ droplets are dispersed through CH$_4$ gas. Figure 5-33, shows the typical liquid-gas separators used in the gas processing industry [36].

![Figure 5-33 Types of Liquid-Gas Separators](image-url)
Centrifugal separation occurs when the centrifugal force of dispersed fluid exceeds drag force by flowing gas. An external source is used to increase the centrifugal force. The filter separator creates a torturous path/obstacle to the liquid droplet, this decreases the velocity of liquid droplets and it eventually falls down to the bottom of the vessel. The Impingement separator uses mist pads to separate liquid droplets by crafting the inertial impaction. The final separator type is the gravity separator which occurs when the gravitation force on liquid droplets exceeds drag force of the gas molecule [37]. This is simple and efficient to separate high gas-liquid ratios. These are oriented either vertically or horizontally. The proposed system is decided to use gravity separation mechanism of vertical orientation.

5.4.1 Design

The gravity liquid-gas separator (LGS) is divided into four sections as shown in figure 5-34. The first section is the inlet device, which reduces the momentum of the inlet stream to impinge liquid droplets on the inlet device then it drops by gravity. The various types of inlet devices commonly used are no inlet device, diverter plate, half-pipe, vane-type and cyclonic. The next section is the gas gravity separation section; it uses the force of gravity to separate the entrained liquid droplet from the gas phase. The third section is liquid gravity separation section, which acts as a reservoir for the removed liquid. The final section is the mist extraction section which utilizes the mist extractor consists of a knitted wire mesh pad, a series of vanes, or cyclone tube [38].

Figure 5-34 Gravity Liquid-Gas Separator [38]
The first step in the design process is to identify the inlet device, no inlet device is chosen to minimize the design complexity. The next step is to determine the required disengagement space for gas gravity separation section. This can be achieved by determining the allowable maximum gas velocity. There are two methods to achieve this object, those are The Sounders – Brown approach (Ks Method) and Droplet settling theory. The Sounders – Brown approach determines allowable maximum gas velocity by balancing forces on liquid droplet whereas, the droplet settling theory determines droplet settling or terminal velocity by following similar force balance. The typical forces acting on liquid droplet are gravity and drag forces. The net force causes the momentum in the same direction. The forces acting on the spherical liquid droplet of diameter ‘Dp’ are

Drag force ($F_d$) by the momentum of a gas molecule is

$$F_d = \frac{C_d A_p \rho_{co2} \nu_{ch4}}{2}$$  \hspace{1cm} (5.56)

Where, $A_p$ is the droplet projected area, defined by $A_p = \frac{\pi}{4} D_p^2$

Gravity force ($F_g$) by the weight of liquid droplet is

$$F_g = (\rho_{co2} - \rho_{ch4}) V_p g$$  \hspace{1cm} (5.57)

Where $V_p$ is the volume of spherical droplet calculated by $V_p = \frac{\pi}{6} D_p^3$

At an equilibrium, the gravity force is equal to drag force, solving equation (5.56) & (5.57) for the maximum gas velocity ($\nu_{max}$) gives

$$V_{gmax} = \sqrt{\frac{4 \ g \ D_p}{3 \ C_d} \left(\frac{\rho_{co2} - \rho_{ch4}}{\rho_{ch4}}\right)}$$  \hspace{1cm} (5.58)

The first term in equation (5.58) is replaced by $K_s$, then the equation is called Sounders-brown’s equation, the equation becomes
\[ V_{gmax} = K_s \sqrt{\frac{\rho_{co2} - \rho_{ch4}}{\rho_{ch4}}} \]  

(5.59)

\[ K_s = a + b P + c P^2 + d P^3 \]  

(5.60)

\( K_s \) is referred as design parameter which can be estimated using the empirical relation, this relation is based on operating pressure (P) and droplet size.

The minimum droplet size is assumed as 100 \( \mu \)m, and the empirical constants for this droplet size are as follows

- \( a = 0.044882 \)
- \( b = 7.24E-5 \)
- \( c = -5.5E-08 \)
- \( d = 1.58E-11 \)

Once the maximum gas velocity is obtained, the next step is to calculate design velocity (\( \nu_d \)) by multiplying selected design factor (percent from 0 to 100 %) to maximum gas velocity.

\[ \nu_d = V_{gmax} V_{af} \]  

(5.61)

The required vessel diameter is determined from design velocity (\( \nu_d \)) and volumetric gas flow rate (\( V_{dotg} \)) as

\[ D_v = \frac{4 V_{dotg}}{\pi \nu_d} \]  

(5.62)

The gas space is assumed to be equal to vessel diameter as per ANSI/API Standard 521. It can be written as
Later, the liquid gravity separation section is designed by assuming the residence time ($t_r$) of liquid on the vessel.

The GPSA Data book [38] suggested the typical residence time for a Natural gas - condensate separation should be within 2 to 5 minutes. The liquid space ($L_l$) from liquid volumetric flow rate ($V_{dott}$) and density ($\rho_l$) as

\[
L_l = \frac{4 V_{dott}}{\pi D_v^2} t_r
\]  

(5.64)

The liquid outlet diameter is calculated from outlet liquid velocity ($V_{lo}$) as

\[
D_{lo} = \sqrt{\frac{4 V_{dott}}{\pi V_{lo}}}
\]  

(5.65)

The gas outlet diameter from outlet gas velocity ($V_{go}$) as

\[
D_{go} = \sqrt{\frac{4 V_{dotg}}{\pi V_{go}}}
\]  

(5.66)

The selection of mist extractor is based on the gas-liquid ratio in the inlet stream. Tamagna et al., [39] suggested that no mist extractor is required for an inlet stream of high gas-liquid ratio. So, the proposed liquid-gas separator is designed with no mist extractor. The final step in LGS design is to determine the required vessel thickness ($t_v$) to hold the pressure which is calculated using ASME Section VIII Division 1 code based on material yield strength ($\sigma_{yield}$), inner vessel radius ($r_l$), Design pressure ($P_d$) and joint efficiency ($E$) as
\[ t_v = \frac{P_d \, r_i}{\sigma_{yield} \, E - 0.6 \, P_d} \] (5.67)

The input parameters required for LGS design are shown in Table 5-19.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate of liquid CO(_2) (mdot\textsubscript{co2})</td>
<td>11 kg/hr</td>
</tr>
<tr>
<td>Mass flow rate of gaseous CH(_4) (mdot\textsubscript{ch4})</td>
<td>4 kg/hr</td>
</tr>
<tr>
<td>Density of CO(<em>2) (\rho</em>{co2})</td>
<td>468.2 kg/m(^3) (Critical density is assumed)</td>
</tr>
<tr>
<td>Density of CH(<em>4) (\rho</em>{ch4})</td>
<td>51.99 kg/m(^3)</td>
</tr>
<tr>
<td>Volumetric flow rate of CO(_2) (vdot\textsubscript{co2})</td>
<td>0.023 m(^3)/hr</td>
</tr>
<tr>
<td>Volumetric flow rate of CH(_4) (vdot\textsubscript{ch4})</td>
<td>0.077 m(^3)/hr</td>
</tr>
<tr>
<td>Volume fraction of CO(_2) (y\textsubscript{co2})</td>
<td>0.23</td>
</tr>
<tr>
<td>Volume fraction of CH(_4) (y\textsubscript{ch4})</td>
<td>0.76</td>
</tr>
</tbody>
</table>

The final parameters of LGS are shown in Table 5-20.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO(_2) liquid droplet size ((D_p))</td>
<td>100 (\mu)m</td>
</tr>
<tr>
<td>Design parameter ((K_s))</td>
<td>0.023 m/s</td>
</tr>
<tr>
<td>Maximum gas velocity ((\nu_{gmax}))</td>
<td>0.068 m/s</td>
</tr>
<tr>
<td>Design gas velocity ((\nu_d))</td>
<td>0.01 m/s</td>
</tr>
<tr>
<td>Vessel diameter ((D_v))</td>
<td>94.95 mm</td>
</tr>
<tr>
<td>Gas space ((L_g))</td>
<td>94.95 mm</td>
</tr>
<tr>
<td>Liquid space ((L_l))</td>
<td>165.87 mm</td>
</tr>
</tbody>
</table>
### Inlet diameter ($D_{in}$)

11.48 mm

### Liquid outlet diameter ($D_{lo}$)

11.48 mm

### Gas outlet diameter ($D_{go}$)

18.56 mm

### Thickness

3.01 mm

### Mass of LGS

0.653 kg

---

CAD modeling of Liquid Gas Separator shown in Figure 5-35.

![2D and 3D model of LGS](image)

**Figure 5-35 2D and 3D model of LGS**

### 5.4.2 CFD multi-phase Analysis

The design is validated by steady-state Multi-Phase Analysis using ANSYS – CFX. This analysis is carried out by importing fluid geometry from CAD software, meshing it to create finite number of elements then assign domain properties and boundary conditions to approximate the solution by solving governing equations using various numerical techniques. Later, the results are analyzed to validate the design.
Figure 5-36 a) Imported fluid CAD geometry with named selections and b) Fine mesh

The Parameters/models are assigned to fluid volume and surfaces. Figure 5-37 shows the ANSYS – CFX (pre) problem setup tree and fluid domain with the boundary conditions, respectively.

Figure 5-37 a) Problem setup tree and b) fluid domain with the boundary conditions

The fluid domain section has various panels to setup multi-phase problem such as basic settings, fluid models, fluid specific models, fluid pairs, initialization. The fluid material, domain properties are assigned in basic settings panel as shown in figure 5-38 (a). The fluid model section is to select the model for analysis. The available models in this panel are multiphase, heat transfer, turbulence, combustion, and thermal radiation. Figure 5-38 (b), shows the models used in the analysis. The fluid specific models are used to assign fluid buoyancy model for individual fluid, density difference model
is chosen as shown in figure 5-38 (c). The fluid pair model defines the interface between gas molecule and liquid droplet as shown in figure 5-38 (d).

The next step is to assign the boundary conditions. As shown in Figure 5-37 (b), the present model has three boundaries such as Mixture inlet, Gas outlet and Liquid outlet. The boundary conditions are tabulated in the table 5-21.
Table 5-21 Boundary conditions

<table>
<thead>
<tr>
<th>Input</th>
<th>Mixture inlet</th>
<th>Gas outlet</th>
<th>Liquid outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow regime</td>
<td>Subsonic</td>
<td>Subsonic</td>
<td>Subsonic</td>
</tr>
<tr>
<td>Mass and momentum</td>
<td>Fluid dependent</td>
<td>Degassing Condition</td>
<td>Fluid dependent</td>
</tr>
<tr>
<td>Inlet CO\textsubscript{2} velocity</td>
<td>0.063 m/s</td>
<td>...............</td>
<td>...............</td>
</tr>
<tr>
<td>Inlet CH\textsubscript{4} velocity</td>
<td>0.206 m/s</td>
<td>...............</td>
<td>...............</td>
</tr>
<tr>
<td>Inlet CO\textsubscript{2} volume fraction</td>
<td>0.23</td>
<td>...............</td>
<td>...............</td>
</tr>
<tr>
<td>Inlet CH\textsubscript{4} volume fraction</td>
<td>0.76</td>
<td>...............</td>
<td>...............</td>
</tr>
</tbody>
</table>

Figures 5-39 & 5-40 shows the velocity vectors of CH\textsubscript{4} gas and CO\textsubscript{2} liquid. It can be observed that the velocity vectors moving in the upward direction in Figure 5-39 and downward direction in Figure 5-40. This indicates the separation of liquid from the gas. The maximum gas velocity is observed in gravity liquid separation section at an interface between liquid and gas. The figures 5-39 & 5-40 also shows the velocity of the CH\textsubscript{4} gas and CO\textsubscript{2} liquid in gas gravity separation section using a probe. It can be clearly seen that maximum velocity is observed for CO\textsubscript{2} liquid at the same location of CH\textsubscript{4} gas.

![Velocity vectors of CH\textsubscript{4} gas](image)

Figure 5-39  Velocity vectors of CH\textsubscript{4} gas
Figure 5-40 Velocity vectors of CO₂ liquid

Figure 5-41 shows the volume fractions of CH₄ gas and CO₂ liquid. The maximum CO₂ volume fraction is observed at the bottom of the vessel whereas, the maximum CH₄ volume fraction observed at the top of the vessel. Based on the velocity vector and volume fraction results, the design is valid.

Figure 5-41 Volume fraction of CH₄ gas and CO₂ liquid
5.5 Light-weight storage tank design and FEA composite analysis

Although the storage tank is not an integral part of the system the design of light - weight storage tank is critical for the system to make it marketable. The aim of this section is to design a light – weight storage tank to store biomethane at 22.06 MPa (CNG quality). The CNG pressure vessels are verified for the proposed design in order to store biomethane at CNG quality. Typical CNG pressure vessel types available in the market are shown in Figure 5-42.

![Diagram showing Types of CNG pressure vessels]

Figure 5-42 Types of CNG pressure vessels

Type I storage tanks are constructed with metals, the typical material used for these type of pressure vessels is CrMo steel. These are less expensive, which has 93 % market share throughout the world. These tanks weigh approximately 1.4 kg/L. Type II storage tanks are constructed by metal liner reinforced with resin impregnated continuous composite fiber overwrap in the hoop direction. Equal loads are shared by the metal liner and composite material. Generally, CrMo or steel/aluminum metal liner with glass fiber composite is used for construction. These vessels share 4% worldwide market and weigh 0.84 kg/L. Type III gas storage tanks are also constructed by the metal liner reinforced with resign impregnated composite fiber but with fully overwrapped in all directions. The typical materials used for the liner and the composite wrap are aluminum and carbon/glass fiber composites. In this, composite material carries 80 % and the metal liner carries 20 % load. The typical specific weight is 0.54 kg/L. Type IV pressure vessel is constructed with resign impregnated continuous
filament with a non-metallic liner typically, high – density polyethylene (HDPE) with carbon fiber composite. These are the lightest CNG vessel weighing 0.39 kg/L [17][40].

5.5.1 Design

The first step in Light – weight storage tank design is to identify the required volume based on the fluid properties inside the tank as shown in table 5-22.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Working pressure (P_w)</td>
<td>22.06 MPa</td>
</tr>
<tr>
<td>Working temperature (T)</td>
<td>300 K</td>
</tr>
<tr>
<td>Gas constant of biomethane (R)</td>
<td>518.3 J/kg*K</td>
</tr>
<tr>
<td>Mass of biomethane (m)</td>
<td>4 kg</td>
</tr>
</tbody>
</table>

The required volume is calculated by

\[ V = \frac{\text{Mass (m)}}{\text{Density (}\rho\text{)}} \]  \hfill (5.68)

The density can be determined by the ideal gas equation as

\[ \rho = \frac{p}{R T} \]  \hfill (5.69)

Table 5-23 shows the weight of each tank type for the proposed system calculated based on the specific volume and required tank volume.
Table 5-23 CNG tank weight

<table>
<thead>
<tr>
<th>CNG tank type</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type I</td>
<td>38.34 kg</td>
</tr>
<tr>
<td>Type II</td>
<td>23 kg</td>
</tr>
<tr>
<td>Type III</td>
<td>14.78 kg</td>
</tr>
<tr>
<td>Type IV</td>
<td>10.68 kg</td>
</tr>
</tbody>
</table>

Though type IV tank is lighter among all the CNG tanks, Type III is chosen for the design. This is because most of the developing countries use Liquid propane gas (LPG) for their household energy needs. Once it compressed the proposed biomethane has almost equal energy as LPG. The typical dry LPG tank weighs 15 to 18 kg with a volume of 27 to 32 L.

Later, the inner radius required for the storage tank is calculated, by selecting the storage tank shape. Generally, the pressure vessels are available in cylindrical and spherical shape. The spherical shape is chosen for the proposed design. These are twice as efficient as cylindrical vessels in terms of wall thickness. It allows half the wall thickness as in the wall of cylindrical pressure vessel [41]. The required radius is calculated from volume (V) using the spherical geometric relation as

\[
r = \left( \frac{3}{4\pi} V \right)^{\frac{1}{3}}
\]

Material selection is vital for the design. The typical materials used for type III tank are aluminum metal liner and Glass/Carbon fiber composite wrap. Generally, the composite is a combination of two or more individual structural material reinforced together to get high strength. The reinforcement of dissimilar materials forms the fiber and these fibers are glued together by high strength epoxy (typically epoxy) to make the composite material. The composite materials are classified into two types such as the Carbon Fiber Reinforcement Plastic (CFRP) and Glass Fibre Reinforcement Plastic (GFRP) [42]. The properties of CFRP and GFRP are shown in Table 5-23.
Table 5-24 Properties of CFRP and GFRP

<table>
<thead>
<tr>
<th>Property</th>
<th>CFRP</th>
<th>GFRP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (ρ)</td>
<td>1518 kg/m^3</td>
<td>2000 kg/m^3</td>
</tr>
<tr>
<td>Yield stress (σ_x, σ_y, σ_z)</td>
<td>1632 MPa, 34 MPa, 34 MPa</td>
<td>1100 MPa, 35 MPa, 35 MPa</td>
</tr>
<tr>
<td>Young’s modulus (E_x, E_y, E_z)</td>
<td>123 GPa, 7.7 GPa, 7.7 GPa</td>
<td>45 GPa, 10 GPa, 10 GPa</td>
</tr>
<tr>
<td>Shear modulus (G_xy, G_yz, G_xz)</td>
<td>5 GPa, 3 GPa, 5 GPa</td>
<td>5 GPa, 3.8 GPa, 5 GPa</td>
</tr>
<tr>
<td>Poisson’s ratio (θ_xy, θ_yz, θ_xz)</td>
<td>0.27, 0.42, 0.27</td>
<td>0.3, 0.4, 0.3</td>
</tr>
<tr>
<td>Minimum burst ratio</td>
<td>2.35</td>
<td>3.65</td>
</tr>
</tbody>
</table>

The Carbon fiber reinforcement plastic (CFRP) is chosen for its high strength and less density over Glass fiber reinforced plastic. The properties of the aluminum liner are shown in Table 5-24.

Table 5-25 Properties of the aluminum liner

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (ρ)</td>
<td>2770 kg/m^3</td>
</tr>
<tr>
<td>Tensile yield strength (σ_ty)</td>
<td>280 MPa</td>
</tr>
<tr>
<td>Tensile ultimate strength (σ_tu)</td>
<td>310 MPa</td>
</tr>
<tr>
<td>Compressive yield strength (σ_cy)</td>
<td>280 MPa</td>
</tr>
<tr>
<td>Young’s modulus (E)</td>
<td>71 GPa</td>
</tr>
<tr>
<td>Bulk modulus (G)</td>
<td>69 GPa</td>
</tr>
<tr>
<td>Shear modulus (K)</td>
<td>26 GPa</td>
</tr>
<tr>
<td>Poisson’s ratio (θ)</td>
<td>0.33</td>
</tr>
</tbody>
</table>

Safety is of primary concern in the design of high-pressure gas storage tank, the failure of storage tanks leads to loss of life, health hazards and property damages. There are various national and international safety standards and codes used for design, testing, inspection, and maintenance. The ASME Boiler Pressure Vessel Section VIII, Division III code is used in the proposed design. The
ASME code indicates minimum metal liner thickness for Type III CNG pressure vessel as 6mm. The pressure capability of a liner is calculated using

\[ P_l = \frac{2 \sigma_{\text{yield}} t_l}{r} \]  \hspace{1cm} (5.71)

The pressure vessel is designed to withstand the burst pressure of the composite material. The burst pressure of the required pressure vessel is calculated using burst ratio (2.35 for carbon composite) of the composite material [43]. The burst pressure of the required pressure vessel is

\[ P_{\text{burst}} = 2.35 P_w \]  \hspace{1cm} (5.72)

The design pressure \( P_c \) of the composite overwrap is calculated from liner pressure capacity which is

\[ P_c = P_{\text{burst}} - P_l \]  \hspace{1cm} (5.73)

The design pressure of the carbon fiber composite overwrap is 34.05 MPa.

The effective thickness of the carbon fibre composite for design pressure can be calculated based on the ASME, Section VIII, Division I.

\[ t = \frac{P_c r}{2 \sigma_c E - 0.2 P_c} \]  \hspace{1cm} (5.74)

Where,

- \( P_c \) is the composite design pressure
- \( r \) is inner radius of the pressure vessel
- \( \sigma_c \) is quasi-isotropic strength of the composite \( \left( \frac{\sigma_x}{2} \right) \)
- \( E \) is the joint efficiency (assumed as 1)
The manufacturing of a composite pressure vessel is different from the typical metal pressure vessel. The filament winding process is widely used in composite pressure vessel manufacturing. In this process filament winding consists of winding resin impregnated fibers of CFRP/GFRP form plies or laminates of some angle (ranging from 45° to 88°) on a rotating mandrel. Mukund Kavekar et al. suggested an optimum 54° winding angle based on FE analysis. The liner thickness is kept constant throughout the spherical pressure vessel but at the polar opening full metal is used because of the practical winding difficulties. The thickness of the polar opening is calculated using

\[ t = \frac{P_{burst} r}{2 \sigma_{tu} E - 0.2 P_{burst}} \] (5.75)

The final properties of the pressure vessel are shown Table 5-25.

<table>
<thead>
<tr>
<th>Properties of the vessel</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>28.19 L</td>
</tr>
<tr>
<td>Inside radius</td>
<td>188.88 mm</td>
</tr>
<tr>
<td>Hydrostatic pressure</td>
<td>28.682 MPa</td>
</tr>
<tr>
<td>Burst pressure</td>
<td>51.84 MPa</td>
</tr>
<tr>
<td>Liner thickness</td>
<td>6 mm</td>
</tr>
<tr>
<td>Pressure capability of liner</td>
<td>17.797 MPa</td>
</tr>
<tr>
<td>Pressure capability of composite</td>
<td>34.05 MPa</td>
</tr>
<tr>
<td>Composite thickness</td>
<td>4.08 mm</td>
</tr>
<tr>
<td>Total thickness</td>
<td>10.08 mm</td>
</tr>
<tr>
<td>Thickness at the polar opening</td>
<td>15.90 mm</td>
</tr>
</tbody>
</table>

CAD modeling of the spherical pressure vessel as shown in Figure 5-43.
5.5.2 FEA composite analysis

The Composite analysis is performed to validate the design using ANSYS workbench 18.2. The figure 5-44 shows the ANSYS project schematic.

![ANSYS project schematic](image)

The components used in the present analysis are ANSYS Composite Pre (ACP-pre), Mechanical model, Static Structural, and ANSYS Composite post (ACP-post). ANSYS Composite PrePost is specially designed to set up the composite model, it allows the user to input the number of plies, ply sequence, winding angle, etc. In this analysis, this component is used to set up the composite part of the pressure vessel. The mechanical model is used to set up the solid part of the vessel. The composite and solid models are merged in Static-Structural component to analyze it for specific boundary conditions.
The first step in ANSYS Composite Pre (ACP-pre) is to assign material data to project schematic from pre-defined Engineering Data Source library. The materials, Aluminum alloy (for metallic liner), Epoxy Carbon UD (230 GPa) wet (for composite laminate), Resin epoxy (to layup the plies) and the Aluminum alloy (for metallic polar opening) are assigned. Figure 5-45, shows the material assigned to ACP-Pre model and material assigned to the mechanical model.

![Figure 5-45 Materials assigned to ACP-Pre and Mechanical model](image)

Geometry is imported from solid works to ANSYS workbench. ACP-Pre requires the surface geometry to set up the composite ply whereas the Mechanical model requires solid geometry. Figure 5-46(a) & (b) shows the pressure vessel surface imported to ACP-Pre and the solid pressure vessel imported to Mechanical Model.
The model is meshed to solve the governing equation. Default fine mesh setup is used in both the models. The mesh is performed only for solid material. A dummy material and thickness is assigned to surface body to avoid errors and this can be corrected by assigning actual metal liner thickness in ACP-pre problem setup step. Figure 5-47 (a) and (b) shows the mesh model of ACP-pre and Mechanical model.

Figure 5-47 a) ACP mesh model and b) Mechanical mesh model
Composite problem setup in ACP-Pre is vital for the analysis as it is aimed to set up laminate ply based on given materials, ply orientation, ply sequence, and winding angle. The first stage in problem setup is to import the material properties to ACP-pre as shown in the top left image of figure 5-48. The next step is to identify and enter fabric thickness in fabric window. The top right image shows the epoxy carbon fabric window. Then the mesh elements are selected from predefined named selection in mesh step. The bottom left figure 5-48 shows the element setup window. Now, the coordinate system is defined for laminate which is shown in the bottom right image in figure 5-48. In the image red arrow shows the laminate wrapping direction, the blue arrow shows the ply direction and the green shows the wrapping angle.

Figure 5-48 ACP problem setup
Once the coordinate system setup is completed the next step is to assign the laminate for each layer by given optimum winding angle. In figure 5-49, the yellow arrow in the top left image shows the laminate wrapping direction, the violet arrow shows the ply direction and the green arrow shows the winding angle. The top right image shows the number of layers on the pressure vessel. The bottom left image shows the composite solid model of five layers (1 metallic layer and 4 composite layers). The bottom right image is the clear view of layers.

Figure 5-49 Composite laminate
Once the composite model is generated in ACP-Pre, the ACP model and Mechanical Model are merged and transferred to Static structural for further analysis. Figure 5-50 shows the solid model of the pressure vessel merged by two solids.

Figure 5-50 ACP-Pre and mechanical model assembly

Boundary conditions and pressures are assigned to solve the FEA model for Von Mises stresses. In Figure 5-51, (a) and (b)boundary conditions and the burst pressure on the pressure vessel.

Figure 5-51 a) Boundary conditions and b) Burst pressure
Once the problem setup is completed, the FEA solver solves the governing equations for Equivalent stress and strain, Total deformation, Maximum and Minimum principal stresses, Middle principle stress, Maximum shear stress, Normal stress, and shear stress. The equivalent stress is important to validate the design. For an acceptable composite pressure vessel design the equivalent stress calculated at burst pressure should be less than the quasi-isotropic strength of the material. The figure below shows the equivalent stress variation in the pressure vessel.

![Figure 5-52 Von-Misses stresses of pressure vessel](image)

From Figure 5-52, it can be observed that maximum stress is located at the contact location. This is because of the imperfections in mesh connection. An accurate mesh model needs to be developed for proper element connection. Though the maximum Von Mises stress is 949.71 MPa, the average Von Mises stress is on the composite structure is 580 MPa which is less than 816 MPa (quasi-isotropic strength of the carbine fiber material). So, the design is valid.
6 SUMMARY AND CONCLUSION

The objective of the current study was to propose a commercial portable biogas purification and storage system to commercialize the biogas produced from household/non-commercial biogas plants. The selection of the purification process was based on the portability of the purification system which is completed based on the available commercial purification processes used in the industrial/commercial biogas plants. The literature review concludes the selection of commercial cryogenic purification process with some modification. The commercial cryogenic process relies on the desublimation of CO\textsubscript{2} for the separation of CO\textsubscript{2} from CO\textsubscript{2} – CH\textsubscript{4} binary mixture whereas the modified cryogenic process was decided to use the condensation of CO\textsubscript{2}. This modification lowers the energy consumption of the system by increasing efficiency, it also gives the flexibility in heat exchanger selection by making it cost effective.

The design of the purification system starts by defining the thermo-physical properties of the biogas and the critical properties of CO\textsubscript{2} – CH\textsubscript{4} binary mixture. Some of the previous works identified that the influence of lower critical condition of gases influences the higher critical condition of gases in a binary mixture. This influence was successfully quantified by modifying the Peng-Robinson equation of state by including the binary interaction parameters of CO\textsubscript{2} – CH\textsubscript{4} proposed by various literature. Later, an experiment was designed to validate the modified Peng – Robinson equation of state to use the quantified data in proposed purification system design. The experiment is performed for the pure CO\textsubscript{2}, 80\% CO\textsubscript{2} – 20\% CH\textsubscript{4}, and 50\% CO\textsubscript{2} – 50\% CH\textsubscript{4}. The data obtained from the experiments were successfully validated the saturated vapor pressures of CO\textsubscript{2} in CO\textsubscript{2} – CH\textsubscript{4} binary mixture obtained from the Peng – Robinson equation of state.

For a preliminary design, a condensation point was chosen in the liquid region of the equation of state of 50\% CO\textsubscript{2} – 50\% CH\textsubscript{4} mixture. The pressure and temperatures of the selected condensation point is 206 K (-67 °C), 5.65 MPa (748.39 psi) respectively. The operating principle of the proposed system is to compress and cool the biogas to condensation point in the liquid region of CO\textsubscript{2} in CO\textsubscript{2} – CH\textsubscript{4} binary mixture then the CO\textsubscript{2} changes its phase from gas to liquid. The liquid CO\textsubscript{2} and the gaseous CH\textsubscript{4} will then be separated and the gaseous CH\textsubscript{4} is further compressed to store it in CNG quality.
components identified in proposed purification system based on the thermodynamic states of the gases explained in Chapter 5.1 are Compressors, Heat exchangers, Liquid – Gas separator, and CH₄ storage tank.

As discussed in the thesis objective the entire purification system (excluding CH₄ storage tank) should be under 15 kg, which a normal person can carry on his/her backpack. All the components were designed to meet this criterion, the mass flow rate of biogas was chosen to be 15 kg/hr (which separates and stores 4 kg/hr methane in CNG quality). Two compressors were decided to use in the system to compress the biogas (compressor 1) and methane (compressor 2) to achieve the required pressure ratio. The major parts of the compressors were designed and validated using FEA structural analysis. The weight of the compressor 1 and 2 we estimated as 3.5 kg and 2 kg respectively.

The proposed purification process requires to cool the biogas from 908.68 K to 206.38 K. It was decided to use two heat exchangers to achieve the required heat dissipation. Chapter 5.3 successfully discussed the design and CFD conjugate heat transfer analysis of heat exchangers. The final heat exchanger (including 1 and 2) assembly weighs 3.7 kg. Liquid-gas separator is the vital part of the system which separates the liquid CO₂ from gaseous CH₄. Chapter 5.4 presented the discussion on design and CFD Multi-Phase analysis of liquid-gas separator. It weighs 0.653 kg. The final component of the system is the CH₄ storage tank. This was designed based on Type III CNG tank; the validation is done by using the FEA Composite analysis. The total weight of the purification system including an estimated piping and control system weights but excluding the storage tank is shown in Table 6-1. The total weight of the system meets the objective with a good margin.

<table>
<thead>
<tr>
<th>Component name</th>
<th>Weight (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressor 1 assembly</td>
<td>3.5</td>
</tr>
<tr>
<td>Compressor 2 assembly</td>
<td>2</td>
</tr>
<tr>
<td>Heat exchanger 1</td>
<td>2.5</td>
</tr>
<tr>
<td>Heat exchanger 2</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Table 6-1 Weight of portable biogas purification system
Table 6-1 – continued

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid gas separator</td>
<td>0.653</td>
</tr>
<tr>
<td>Piping and control system</td>
<td>2</td>
</tr>
<tr>
<td>Total weight</td>
<td>11.853</td>
</tr>
</tbody>
</table>
7  FUTURE SCOPE

The present work successfully identified and proposed a portable purification and storage system for biogas. The preliminary design of the components is completed to meet the design criteria based on various ideal assumptions. This work can be extended to test the proposed cooling system and identify the best alternative cooling methods. Once the cooling system test completed, the next step is to build and test the prototype to validate the purification system design experimentally. The alternative purification methods could also verify for the final product.
REFERENCES


[29] A. Morriesen and C. J. Deschamps, “Experimental investigation of transient fluid flow and


[34] I. S. O. Designation, “Compressor oils.”


