Nazarbayev University School of Engineering and Digital Sciences
Chemical and Materials Engineering Department
CHME 400 Capstone Project

Capstone Project II
Report 4

Using syngas for production of methanol with energy integration

Group members: Gulnur Sultan
Bakytzhan Ibraimuly
Aktoty Zagyppar
Dana Yerkhan
Tlek Bulekchurin

Supervisors: Professor Yanwei Wang
Professor Stavros Poulopoulos

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I. Process Introduction

1.1. Introduction

Methanol is a crucial raw material for the future energy and fuel industries as well as the chemical sector. Syngas is the primary source of methanol produced nowadays. The objective of the capstone project is to build a chemical plant for the production of commercial methanol. The factory, which will be situated in Kazakhstan, will turn syngas into methanol. Methanol's main applications stem from its significance in the synthesis of chemicals. First, formaldehyde, acetic acid, methyl tert-butyl ether (MTBE), and dimethyl ether (DME) are all produced using methanol as a feedstock (Lücking, 2017).

There are now 110 million metric tonnes of installed methanol production capacity worldwide, in order to supply the yearly demand of 70 million metric tonnes (Lücking, 2017). Talking about Kazakhstan, it has 2 big oil and gas plants which consume methanol. There is a methyl tert-butyl ether (MTBE) production plant by Shymkent Chemical Company and a tert-amyl methyl ether production plant by Atyrau Oil refinery. In comparison to 2021, the methanol demands of both plants have increased to 4.8 kT/yr and 3.4 kT/yr, respectively, in 2022 (Казахстан Увеличивает Закупки Метанола, 2023). This trend provides a crucial insight: Kazakhstan's methanol market is evolving similarly to those of the major methanol producing nations, such China, the United States, or Russia, where methanol is primarily utilized for production and is expected to see an increase in societal use in the years to come.

The current effort starts with the selection of the manufacturing process through comparison of all intriguing commercial ways for producing methyl alcohol. The project will look at the toxicity-based health and safety assessments of the chemicals as well as an analysis of the economic data. A thermodynamic study will be taken into account to identify the chemical and physical characteristics of the materials utilized in the process. Last but not least, the Process Flow Diagram (PFD) will include operating unit information for each phase and be utilized later to calculate the material balance.

The main goals to be pursued are:

- Literature review on manufacturing options;
- Selection and justification of a production rate;
- Analysis of the properties of pure components and mixtures;

- Analysis of the security measures of the selected process and involved chemicals;
- Designing the process flow diagram and major/minor equipments

1.2. General physical and chemical properties of methanol

Methanol (CH_3OH) also known as methyl alcohol and methyl hydrate is a C1 building block widely used in the chemical industry. It is a colorless, volatile liquid that has a slightly sweet but strong scent similar to ethanol. Methanol has a molecular weight of 32.043 g/mol and octane number equal to 113. Also, it consists of methyl and hydroxyl groups, making the methanol molecule polar. Hence, it is completely soluble in water and organic solvents, and slightly soluble in fat or oil (Dalena et al., 2018).

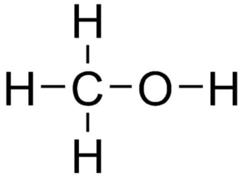


Figure 1.2.1. Molecular formula of methanol.

Table 1.2.1. Identifiers of methanol.

IUPAC name	Methanol
CAS number	67-56-1
Synonyms	methyl alcohol, carbinol
Molecular formula	CH_4O
InChI	InChI=1S/CH4O/c1-2/h2H,1H3

Table 1.2.2 Physical and chemical properties of methanol.

Property	**Value**	**Reference**
Boiling point	64.7 °C	(Maryadele J. O’Neil (Editor), 2013)
Autoignition temperature	440-464 °C	(National Fire Protection Association :: NFPA, 2010)

Melting point	-97.8 °C	(Maryadele J. O’Neil (Editor), 2013)
Flash point	9.7 °C (closed cup)	(*Product Safety*, n.d.)
Flash point	15.6 °C (open cup)	(*Environmental Health Criteria Monographs (EHCs)*, n.d.
Liquid density at 20°C	786.3 kg/m^3	*(Methanol - Density and Specific Weight vs. Temperature and Pressure*, n.d.)
Relative vapor density	1.11	(Maryadele J. O’Neil (Editor), 2013)
Vapor pressure at 20°C	12.9 kPa	(*METHANOL*, 2018)
Viscosity at 25°C	0.544 mPa	(*HANDBOOK OF CHEMISTRY and PHYSICS*, 2014)
Specific heat at 20-25 °C	2.12-2.53 kJ/kg*K	(Maryadele J. O’Neil (Editor), 2013)

1.3. Uses and applications of methanol

The primary uses of methanol come from its importance in chemical production. Firstly, methanol is used as feedstock for production of formaldehyde, acetic acid, methyl tert-butyl ether (MTBE), dimethyl ether (DME), methyl methacrylate (MMA), methyl and vinyl acetates, methylamines, melamine resin, ethylene, and propylene.

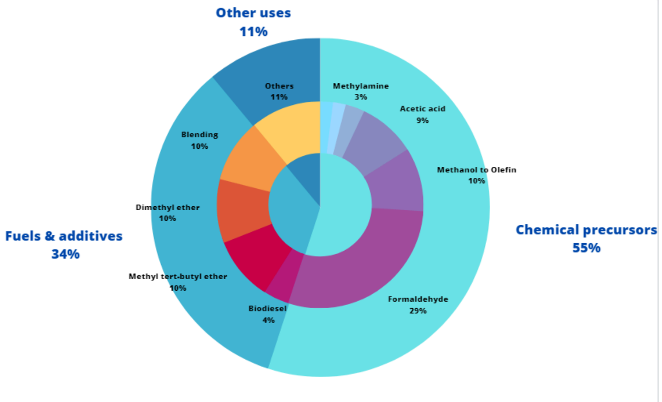


Figure 1.3.1 Uses of methanol 2021 (Sepahi & Rahimpour, 2023).

As it can be noticed from the picture, a major part of methanol is used to produce formaldehyde. A chemical that is used as a germicide, fungicide, and disinfectant and as a preservative in mortuaries and medical laboratories. It was initially obtained in 1910 by reacting air with methanol under 600°C on a silver catalyst.

$$CH_3OH \rightarrow CH_2O + H_2 \qquad (1.3.1)$$

It was an endothermic reaction with enthalpy change of $\Delta H = \ - 84\, kJ/mol$ and required a very high temperature. Therefore, in 1931 a new process with lower temperatures and 90% yield by Reuss et al. was offered. The process's enthalpy change was $\Delta H = \ - 159\, kJ/mol$ (Formaldehyde, Reuss).

$$CH_3OH + \frac{1}{2}O_2 \rightarrow CH_2O + H_2O \qquad (1.3.2)$$

Other than formaldehyde, recently, the production of dimethyl amides takes a valuable 10% of methanol usage. The addition of DME into the fuel decreases the amount of NO_x and engine noise. DME production reaction from methanol is shown below (Sepahi & Rahimpour, 2023).

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \qquad (1.3.3)$$

Other than that, the product can be used as a fuel for vehicles and other machinery. It can also be combined with gasoline to create the efficient fuel methyl tertiary butyl ether (MTBE), which has the potential to emit fewer greenhouse gasses than regular gasoline.

1.4. Selection of the manufacturing process

The extensive literature review was completed in terms of the manufacturing options, as there are many variables in it. The high-pressure method was not in favor, as it was operating on the very energy-consuming conditions, such as the 250-350 bar and 320-450◦ C (Tijm et al., 2001).Thus, the low-pressure method was chosen because it is more modern and widely-used, along with the manufacturing benefits of consuming less energy. The main significant point is that the low-pressure method does convert less amount of syngas in one pass, so it requires the recycle loop and proper separation technique. The thermodynamic model SRK was chosen to do the Aspen calculations.

CuO, ZnO and Al_2O_3 a based catalyst has been chosen due to being the most effective option nowadays. Catalysts with different components are present, but the CuO, ZnO and Al_2O_3 the mixture showed the best results and has necessary research results to validate the choice (Tijm et al., 2001).Separation of raw methanol has also been concluded to be the important part of the whole process. The three-column distillation process was chosen, as it is the most effective way of achieving the most purity out of the methanol product, with the affordable costs.

The main goal of the chemical plant is to produce the methanol with the purity exceeding 99.85 wt%, so the chosen process of Lurgi, the separation method, and catalyst ensures that this goal is achieved, the necessary production rate is performed, he nce the demand for the local methanol production will be fulfilled.

1.5. Construction Materials

In the manufacture of methanol, carbon steel or low-molybdenum steels are typically utilized as building materials. Stainless steels are typically employed during the methanol condensation stage since organic acids are likely to be encountered at that stage. Small amounts of diluted caustic soda can also be added to the distillation phase to minimize damage caused by acids.

Stainless steels are typically used in equipment that operates in environments where iron pentacarbonyl production is probable. This holds true for heat exchangers, for instance. Because iron pentacarbonyl breaks down at the temperatures required for the production of methanol, contamination with it should be avoided. The catalyst is poisoned by iron deposits, which further promote the production of higher hydrocarbons, or waxy products (Ott et al., 2012).

II. Process summary

2.1. Existing manufacturing processes

There are several ways of synthesizing methanol. This chapter reviews the classification of the processes by the applied pressure, namely the BASF and Lurgi processes, which are high-pressure and low-pressure methods respectively. Two methods differ in the operating pressure, catalyst choice, and conversion rates (Abrol & Hilton, 2012).

The primary industrial technique for methanol production involves generating synthesis gas through the steam, oxygen vapor, or carbon dioxide conversion of natural gas. This is followed by methanol synthesis, where carbon monoxide and carbon dioxide are reduced using hydrogen in the presence of a catalyst. Adding carbon dioxide to the steam conversion of natural gas (steam-carbon dioxide conversion) yields a more favorable balance of reactants in the initial gas mixture for methanol synthesis. (Tijm et al., 2001)

The main stages of methanol production are:

- Syngas (synthesis gas) production
- Conversion of syngas to methanol
- Distillation of methanol

Methanol can be produced from both CO and CO_2 syngas. Equations below show the stoichiometry of these reactions and reaction enthalpy.

$$CO + 2H_2 \rightleftarrows CH_3OH \qquad \Delta H_{298K} = -90.77 kJ\,mol^{-1} \tag{2.1.1}$$

$$CO_2 + 3H_2 \rightleftarrows CH_3OH + H_2O \qquad \Delta H_{298K} = -49.16 kJ\,mol^{-1} \tag{2.1.2}$$

Carbon monoxide and carbon dioxide react with hydrogen to form methanol and water. These reactions are reversible, homogeneous, exothermic and proceed with a decrease in volume. Therefore, in accordance with the Le Chatelier principle, the equilibrium of the reaction can be shifted towards the yield of the product when the pressure increases and the temperature decreases (Sepahi & Rahimpour, 2023). However, since the reaction rate is extremely low at low temperatures, heating of the reaction mixture is necessary. In addition, endothermic reverse water gas shift reaction (RWGS) also happens.

$$CO_2 + H_2 \rightleftarrows CO + H_2O \qquad \Delta H_{298K} = 41.21 kJ\, mol^{-1} \tag{2.1.3}$$

In case of Cu catalyst usage during methanol synthesis, CO is more desired than CO_2. However, it would not be possible to use only CO as a feed because of kinetic reasons a minimum 2.5-3.5% of CO_2 has to be present as a raw material. Consequently, the more CO and the less CO_2 is contained in the synthesis gas, the more efficient the conversion is. Also, it is important to calculate the stoichiometric ratio of the syngas as it affects the reaction of methanol synthesis and conversion rate. Ideal value of SN for synthesis of methanol is little above two, showing the excess of hydrogen.

$$SN = \frac{[H_2]-[CO_2]}{[CO]+[CO_2]} \tag{2.1.4}$$

All reactants convert to methanol if SN equals to 2. Carbon dioxide and carbon monoxide are limiting components if SN is more than 2 and hydrogen is limiting reactant if SN is less than 2 (Kuipers, 2014). Side reactions during production cause useless consumption of synthesis gas and increase the cost of methanol production.

The catalyst used for the synthesis of methanol should have high selectivity, i.e. accelerate the formation of methanol as much as possible while suppressing side reactions. There are various catalysts for the synthesis of methanol. The best catalysts turned out to be the main components of which are zinc oxide or copper oxide. Methanol synthesis catalysts are very sensitive to catalytic poisons, so the first stage of the process is the purification of gas from sulfur compounds. Sulfur compounds poison zinc-chromium catalysts reversibly, and copper-containing catalysts irreversibly. It is also necessary to thoroughly clean the gas from iron carbonyl, which is formed as a result of the interaction of carbon monoxide with iron equipment. On the catalyst, iron carbonyl decomposes with the release of elemental iron, which contributes to the formation of methane. The methanol production process is carried out either on a zinc-chromium catalyst at a pressure of 300 bar, or on a low-temperature copper-containing catalyst at a pressure of 50 bar. Zinc-chromium catalyst operates in the temperature range of 370-390℃, copper–containing - 220-280℃. That is, the process of methanol production is heterogeneous-catalytic. The limiting stage is the adsorption of hydrogen on the surface of the catalyst (Tijm et al., 2001).

There are several reactors in use for methanol synthesis: cooled reactors, adiabatic reactors, quench reactors and boiling water reactors (BWR) (Sepahi & Rahimpour, 2023).

2.2. High pressure process

The high pressure method remained the dominant technology for over 45 years. This type of the process was developed by German engineers from European multinational largest chemical producer company Baden Aniline and Soda factory (BASF) in 1923. It operated at up to 250-350 bar pressure and 320–450 °C temperature and hence consumed a lot of energy (Tijm et al., 2001).

2.3. Low pressure process

Originally, the synthesis gas used was derived from German coal/lignite, which was contaminated with chlorine and sulfur, leading to the development of a poison-resistant zinc oxide/chromium-based catalyst (ZnO/Cr2O3). Although copper-based catalysts were initially tested, they did not yield satisfactory results. In the 1960s, Imperial Chemical Industries (ICI, now Synetix) improved the copper-based catalyst technology. They discovered that zinc was an ideal dispersant for copper, which enhanced the catalyst's reactivity and allowed for the operation under less severe conditions, known as the "low pressure" method. This method operated at pressures between 35–55 bar and temperatures of 200–300 °C. Generally, the low-pressure process is considered superior to high-pressure methods as it reduces both the cost of methanol production and the consumption of raw materials. However, it requires much larger reaction vessels.

Currently, methanol synthesis typically occurs under low pressures, sometimes approaching those used in steam reforming to produce synthesis gas. These low-pressure methods consume significantly less energy due to the high costs associated with synthesis gas compression. Catalysts are essential for accelerating reactions, particularly the shift reaction that maximizes the use of synthesis gas. Methanol converters need to operate within a temperature range of 200–300 °C to ensure the catalysts remain active and to effectively utilize the heat of the reaction, despite the equilibrium favoring lower temperatures. The highly exothermic nature of these reactions makes heat removal a critical component of the process.

Low pressure methods generally convert only a small fraction of the synthesis gas in each pass, typically around 10%, as higher pressures favor greater conversion. To achieve suitable yields, these methods use a recycle loop along with a purge gas to eliminate contaminants that would build up over time. The volume of the purge depends on the stoichiometric ratio of the reactants in the synthesis gas. For example, absorbing or adsorbing CO2 may be necessary to remove excess carbon oxides when there is an abundance in the environment. Conversely, if there is an excess of hydrogen, water may be required for its removal. CO2 injection is also considered in other scenarios.

In low-pressure methanol synthesis, the current catalysts used are copper oxide and zinc oxide, with aluminum oxide acting as the carrier. The proportions of these components vary from one manufacturer to another, with CuO usually ranging from 40 to 80%, ZnO from 10 to 30%, and Al2O3 from 5 to 10% (Tijm et al., 2001).

The primary goal of reactor design is to ensure the ideal temperature profile while minimizing the reactor volume to the greatest extent possible. Here is the list of key technological solutions that are currently in use. According on the temperature profile and how the heat transfer is controlled, the low pressure methanol reactor designs can generally be divided into the following categories:

1. Adiabatic reactor, ICI (now Johnson Matthey) technology,
2. Quasi-isothermal reactor as in the boiling water reactor (BWR) as in Lurgi plants
3. Double - reactor solution, MegaMethanol, formerly a Lurgi solution, nowadays the AirLiquide technology.

The reactor is the most significant piece of equipment in every chemical process. The reactor is built to enable effective temperature control because the synthesis of methanol involves globally exothermic processes. To maximize the process's economics, heat must be effectively evacuated and possibly recycled. To keep the expenses of downstream separation to a minimum, high conversion per pass is necessary. The main differences among them are related to the reactor design and catalyst arrangements. There are several types of reactors (Bozzano & Manenti, 2016).

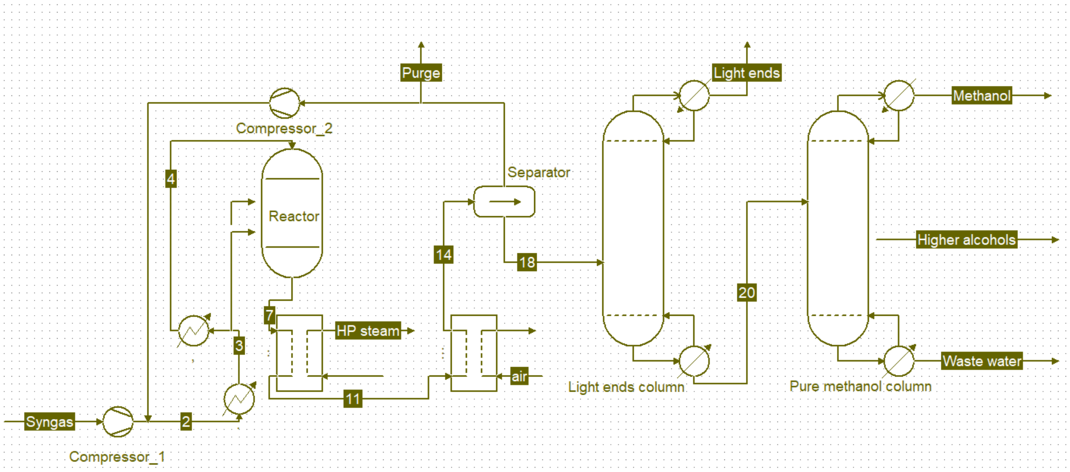
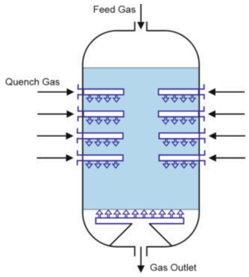
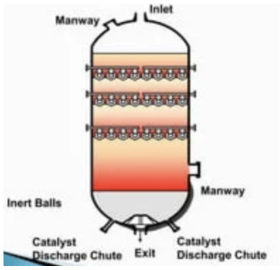
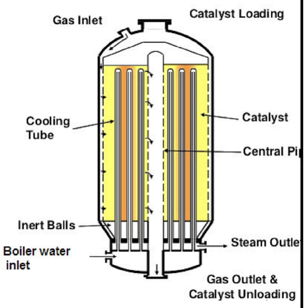
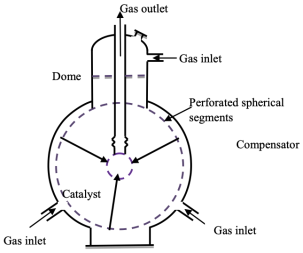
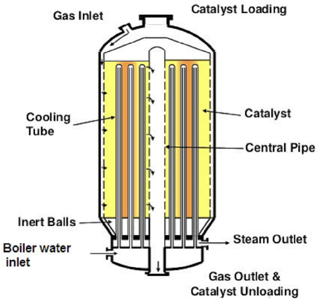


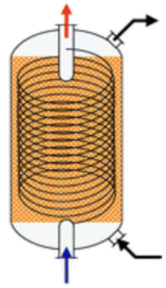
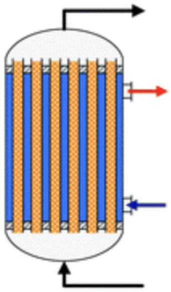
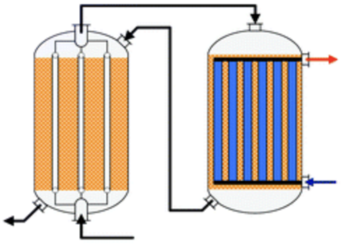
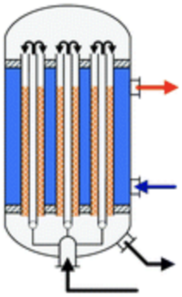
Figure 2.3.1 A flow diagram presenting the Lurgi low pressure methanol synthesis (Matzen, 2016).

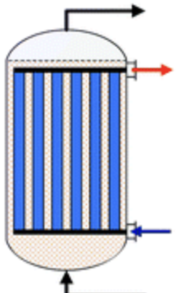
Table 2.3.1. demonstrates all of the available commercial solutions with their associated key features. As noted by Bozzano and Manenti, Lurgi (taking into account both the BWR and MegaMethanol) and ICI technologies account for more than 85% of the installed reactors globally (Bozzano & Manenti, 2016).

Table 2.3.1. Types of reactors for methanol production.

Company	Features	References
Johnson Mattley  	● Quench reactor ● Pressure between 50-100 bar ● Temperature 270 ℃ ● Flow: radial and axial ● Small scale application (less than 2200 t/d)	-Wernicke et al. -Bozzano and Manenti -Dieterich et al.
ICI	● Improved version of Johnson Mattley ● Improved quenching ● Catalyst beds are separate ● 20% increased methanol	Graaf and Beenackers Bozzano and Manenti Dieterich et al.

	production	Westerterp et al.
Haldor Topsoe and Casale SA 	● Lessening of the pressure ● (Haldor) Gas quench reactor and (Casale SA) boiling water	Wernicke et al. Tijm et al. Bozzano and Manenti Dieterich et al.
Kellogg Brown and Root (KBR) 	● Shape is spherical ● Flow is radial ● Small pressure drop ● Series of adiabatic, fixed bed reactors	Bozzano and Manenti Dieterich et al. Tim et al. Westerterp et al.
Toyo Technology Company 	● Radial flow ● Intermediate cooling ● Temperature control is optimal ● Small pressure drop	Bozzano and Manenti Dieterich et al. Hirotani et al. Tim et al.

Linde 	● Axial flow ● Cooling is indirect	Lembeck Bozzano and Manenti Dieterich et al.
Lurgi (multitubolar BWR) 	● Producing steam ● Simple design ● Low manufacturing costs	Haid and Koss Westerterp et al.
Lurgi (Mega Methanol) 	● BWR and GCR reactors ● BWR is smaller ● Low recycle ratio	Keramat et al. Wernicke et al. Bozzano and Manenti Dieterich et al. Ott et al.
Mitsubishi Heavy Industries 	● Integrated BWR and CGR ● Double walled pipes	Wernicke et al. Bozzano and Manenti Tijm et al.

AirProducts (LPMEOH - Liquid phase methanol synthesis) 	● Mild pressure 30-50 bar ● Low production volume	Dieterich et al. Hansen and Heilund Nielsen Tijm et al.

Despite the possibility of slurry technology being a substitute in the near future, fixed-bed technology currently dominates the market (Dieterich et al., 2020). The production capacity, distribution/location of the catalyst, and heat management are the factors that set the various technologies apart from one another. The majority of these technologies make use of indirect cooling using boiling water (BW). If the tube bundle is appropriately built, this indirect cooling system ensures efficient heat dissipation and, in theory, a quasi-isothermal interior temperature profile preventing hotspots (Hansen & Højlund Nielsen, 2008), (Manenti et al., 2011). The MegaMethanol uses the pre-heater's gas indirect cooling to reduce the size of the main reactor (BWR).

Methanol synthesis is enhanced by placing the catalyst on the tube shell side, a setup utilized in the megaMethanol technology for large-scale facilities. Mitsubishi and Toyo technologies incorporate a dual-pipe bundle system that combines boiling water cooling with petrol cooling. This arrangement efficiently manages reaction heat by simultaneously preheating the reactants using a gas-gas heat exchanger and generating water vapor through a gas-transition phase liquid heat exchanger. In this design, the catalytic bed is located in the annular section of the double-pipe tube (Tijm et al., 2001). Meanwhile, the ICI approach employs direct quenching, where the reactor passes through several short catalytic fixed beds as part of the quenching process.

Two key benefits of the direct quenching design are the temperature lowering and equilibrium shifting. The thermodynamic equilibrium involved in the synthesis of methanol is positively impacted by both effects (Hansen & Højlund Nielsen, 2008), (Manenti et al., 2011). Radial reactors enable lower pressure drops and more compact units when operations are taken into account. As various works have demonstrated, this also results in a simpler reactor and process scale-up. Although the choice of reactor technology is mostly influenced by plant size. The Lurgi single-stage technology (BWR) is the most economically advantageous solution for small plants (2200 ton/day), whereas MegaMethanol and ICI solutions compete for best outcomes for large plants (>7000 ton/day).

The Lurgi reactor was identified as the most appropriate choice for the local methanol production**.** It is based on the tubular reactor design, where the gas flows in the axial direction (Dieterich et al., 2020). The most important component is the tubular reactor, which is similar to the shell and tube heat exchanger, due to having carbon steel tubes. Catalyst is contained at the screen at the bottom, where the tubes are closed by the hinged grid. The space between the tubes contains the boiling water, which is beneficial for the catalyst, as it could contain the nearly constant temperature at all times (Chatterjee et al., 1981). The reactor has a shell-tube structure, which allows the boiling water flowing into the shell side to compensate for the heat coming from the tube side. Even though the overall reactor structure is more complicated, due to the shells and tubes, it serves as the great tool for heat integration of the catalytic beds (Cui & Kær, 2020). Following are the main characteristics of the Lurgi reactor (Dieterich et al., 2020).

Table 2.3.2. Key features of the Lurgi reactor for methanol production

Licensor	**Reactor type**	**Flow**	**Catalyst location**	**Heat exchanger**	**Pressure, bar**	$T_{outlet/peak}$ (°C)	**Capacity (ton/day)**
Lurgi	BWR	axial	tube side	tubular	50-100	250/270	<2200

Although kinetics always favors higher temperatures, methanol synthesis is thermodynamically favored at low temperatures. Therefore, it was concluded to use the Lurgi reactor and its conditions in the further investigation.

2.4. Catalyst types in different processes

Nearly all of the methanol production plants nowadays use catalysts to enhance the process. Although different companies have the catalysts which differ in their composition, most of them are based on the CuO, ZnO and Al_2O_3. The proportion vary for CuOfrom 40 and 80%, for ZnO it is 10 and 30%, and for Al_2O_3 it is 5 to 10% (Tijm et al., 2001). Historically, the different catalyst options were tested, so they should be discussed and best should be chosen.

As the CuO, ZnO and Al_2O_3isthe most efficient composition for the catalyst, the main goal is to choose the right proportion of the components, hence, the alternatives will represent the different way of the preparation. The chosen method is the low-temperature one, so the alternatives will represent the catalysts prepared on higher temperatures (Yang et al., 2008).

Table 2.4.1. Methanol synthesis with catalysts calcined at the different temperatures.

Temperature of the calcination (K)	**Diameter of the Cu (nm)**	**Conversion (%)**		**Productivity** $mmolkg^{-1}h^{-1}$	**Selectivity (%)**
		CO	CO_2	CH_3OH	
No calcination	22	14.4	-2.4	191.9	96.4
573	38	9.8	-3.5	125.6	93.9
623	42	9.0	-6.4	106.7	91.4
673	43	8.8	-6.5	66.7	84.5

Table 2.4.2 displays the similar results, but in this case, the precursors were reduced at the various temperatures (Yang et al., 2008). Here, catalysts were not calcined, but reduced to the various temperatures. When reducing to the 220℃, catalyst showed the best conversion for CO and CO_2. Due to the increase in particle diameter and subsequent decrease of the copper surface

area, the methanol productivity is decreased while the temperature increases from 220℃ to 220℃ and 240℃.

Table 2.4.2. Methanol synthesis with catalysts reduced at the different temperatures.

Temperature of the calcination (K)	**Diameter of the Cu (nm)**	**Conversion (%)**		**Productivity (** $mmolkg^{-1}h^{-1}$)	**Selectivity (%)**
		CO	CO_2	CH_3OH	
473	11	10.1	-3.7	159.4	94.9
493	22	14.4	-2.4	191.9	96.4
513	34	10.6	-4.3	173.9	95.2
533	42	10.6	-4.5	155.2	92.4

Table 2.4.3. shows how the copper loading influences the properties (Yang et al., 2008). The results clearly show that 5 wt.% of Cu loading is the most reliable one, which showed better conversion, productivity, and selectivity. The surface area was calculated by the Brunauer-Emmett-Teller method (Yang et al., 2008).

Table 2.4.3. Methanol synthesis with catalysts with the different cuprum loading.

Cu (wt.%)	**BET** (m^2/g)	**Conversion (%)**		**Productivity (** $mmolkg^{-1}h^{-1}$	**Selectivity (%)**
		CO	CO_2	CH_3OH	
3	110	6.1	-6.7	100.0	91.6

5	103	14.4	-2.4	191.9	96.4
7.5	97	9.8	-4.9	150.7	96.2
10	92	9.5	-5.9	162.3	95.7

And finally, Table 2.4.4. presents how the Zu/Cu molar ratio changes the parameters (Yang et al., 2008). 1/1 molar ratio showed better results in each property tested, hence, it can be concluded that this ratio should be implemented further.

Table 2.4.4. Methanol synthesis with catalysts with the different Zu/Cn molar ratios.

Zn/Cu (mol)	**BET** (m^2/g)	**Conversion (%)**		**Productivity** ($mmolkg^{-1}h^{-1}$	**Selectivity (%)**
		CO	CO_2	CH_3OH	
0	112	11.8	-10.8	90.4	86.3
1/2	105	14.2	-24.4	118.7	92.1
1/1	103	14.4	-2.4	191.9	96.4
2/1	93	13.4	-19.6	153.6	96.1

Analyzing all of the data, it was concluded that the most efficient catalyst prepared by the coimpregnation method, is the one where precursors are not calcined and reduced to the 220℃, as the surface area of the copper was increased. The 5% copper loading and ratio of 1/1 for the Zn/Cu, as it was suggested by Yang, et.al., 2007 will be used. CO conversion became stable at 14.4%, while CO_2 was at -2.4%, overall stability was analyzed by the time on stream set to 30 hours (Yang et al., 2008).

2.5. Separation of raw methanol

To achieve the necessary purity of methanol produced from syngas, distillation is the predominant separation method employed. Its extensive use in the methanol production process is attributed to its efficiency in separating methanol from other components to reach the desired purity levels. Methanol, with a lower boiling point of 64.65 (Methyl Alcohol Phase Change Data, n.d.) compared to most components in syngas, provides a significant advantage. Distillation allows for the production of high-purity methanol by offering precise control over the separation process. Adjustments in temperature and pressure settings enable the production of methanol with purity levels exceeding 99% (Zhang et al., 2010).

The distillation process typically utilizes two or more columns or trays to separate methanol from any remaining impurities or byproducts. It is well-suited for large-scale industrial operations, making it ideal for industrial-scale methanol production. The columns in a distillation setup can be designed for continuous operation, and spent solvents can be regenerated, enhancing the process's overall efficiency. Currently, the industry focuses on optimizing certain aspects of distillation, such as column diameter, to reduce overall costs (Hajavi et al., 2016). The typical setup includes a two-column distillation structure.

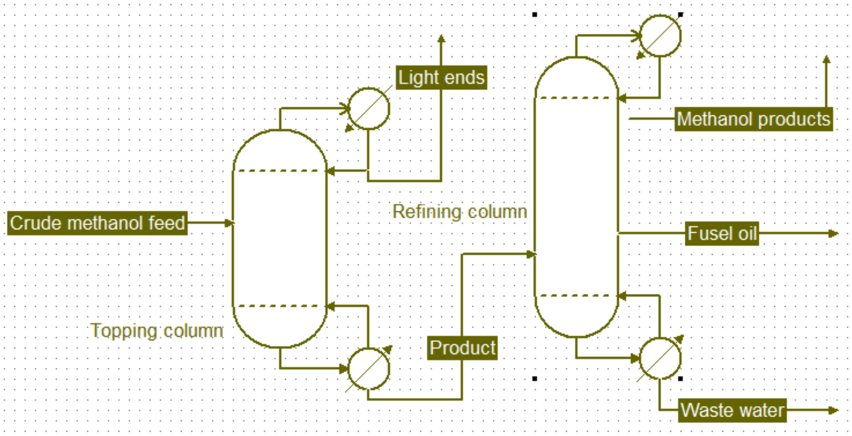


Figure 2.5.1. Two-column distillation structure at the beginning of the Low-Pressure method.

Later on, Lurgi proposed the improved variation, which consisted of three columns having different functions. It was structured to have a pre-run column, higher-pressure column, and an atmospheric column.

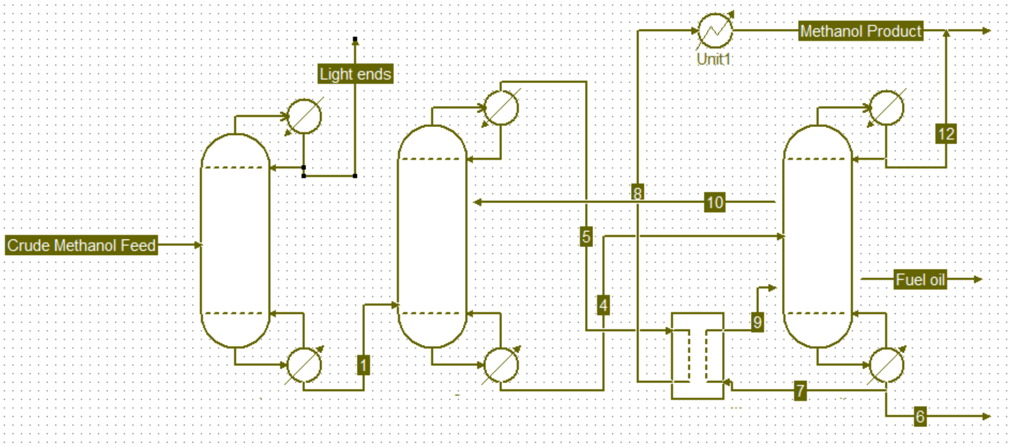


Figure 2.5.2. Three-column double-effect distillation structure.

In a three column structure (Fig 2.5.3), crude methanol is purified by pre-run column C1, high pressure column C2, and atmospheric column C4. The columns C1 and C4 work at a pressure level above the atmospheric pressure while C2 pressurized to 5 - 8 bar (Zhang et al., 2010).

First, methanol is pre-heated and goes into column C1 at the top of the section where the methanol vapor produced in the heat exchanger performs a stripping action to remove the lighter components such as DME or residual gasses. After the bottom product of C1 is pressurized and heated it goes to C2,where approx 40-50% methanol product comes out overhead (Zhang et al., 2010). Then the bottom product of column C2 goes to column C4, from where the residual methanol comes out as an overhead product, and wastewater is taken out as the bottom product. Mid-boiling impurities (in particular ethanol) pass out as a bypass below the feed stage. The overhead vapor of the higher pressure column C2 is used to heat the sump of column C4.

In general, the methanol concentration in the bottom of the atmospheric column wastewater is within the range of 0.01%-0.1%, which does not meet effluent requirements. Moreover this side-stream of the C4 column is also full of methanol. The majority of the methanol remaining at the bottom and exiting with the side-stream exiting from column C4 is collected at column C5 as the overhead. Fusel oil is taken off in a side stream, and wastewater comes out from column C5 as a bottom product.

In comparison to the normal two columns plan, the four-column plan could save about 30% of energy.

However, with all the advantages of the four-column design, there remain several drawbacks. Firstly, Temperature in the bottom of the pre-run column C1 is less than that of the bottom of the atmospheric column C4. While column C4 uses the overhead vapor from column C2's pressure (40 bar) as the heat source, column C1 on the other hand utilizes the 5 bar streams as the heat source. Secondly, Column C2's energy consumption, accounting for around 40% of the total consumption, is slightly excessive as well as the steam consumption of its reboiler (Zhang et al., 2010).

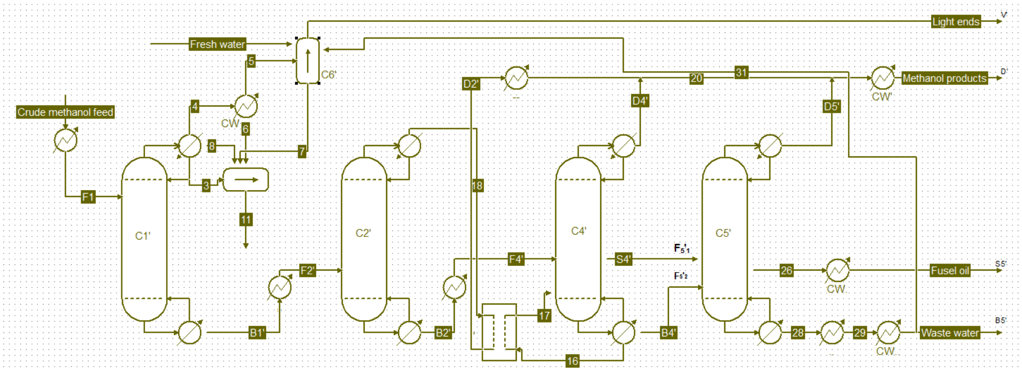


Figure 2.5.3. Four-column double-effect distillation structure. (C1 , pre-run column; C2 , higher-pressure column; C4 , atmospheric column; C5 , recovery column; C6 , water wash column; AC, air-condenser; SW, saturated steam; CW, cooling water; F , feed; D , overhead product; B , bottom product; S , side-draw; V , light ends).

Thus, considering all of the pros and cons of the different column arrangements, the three-column distillation method is the most favorable one, as it allows to get the product of the desired purity, relatively energy-effective, and will result in less costs than the four-column arrangement.

According to the catalyst research, it was identified that even though the 1/1 molar ratio of CuO and ZnO showed some more productivity, there is a limited choice of catalysts which are actually composed in this way, hence, a more convenient and commonly used 2/1 ratio was used.

The most reliable choice will be the MK-121 catalyst from Topsoe, based on the optimized copper dispersion, with the loading density of 1200 kg/m^3 (Dieterich et al., 2020).Following are the characteristics of the chosen catalyst:

Table 2.5.1. MK-121 catalyst specifications

Catalyst	Composition $CuO/ZnO/Al_2O_3(wt\%)$	Temperature, $^{\circ}C$	Pressure, bar
MK-121	55/21-25/8-10	200-310	39-122

2.6. Process description, Process Flow diagram

The production of methanol consists of 2 main processes which includes the production of methanol from syngas and purification of obtained crude methanol. This chapter will cover process descriptions and process flow diagrams.

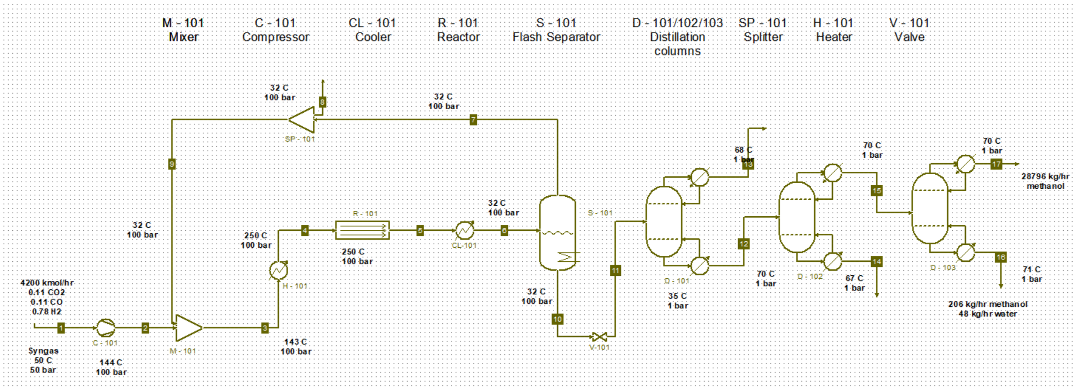


Figure 2.6.1. The Process Flow Diagram of methanol production

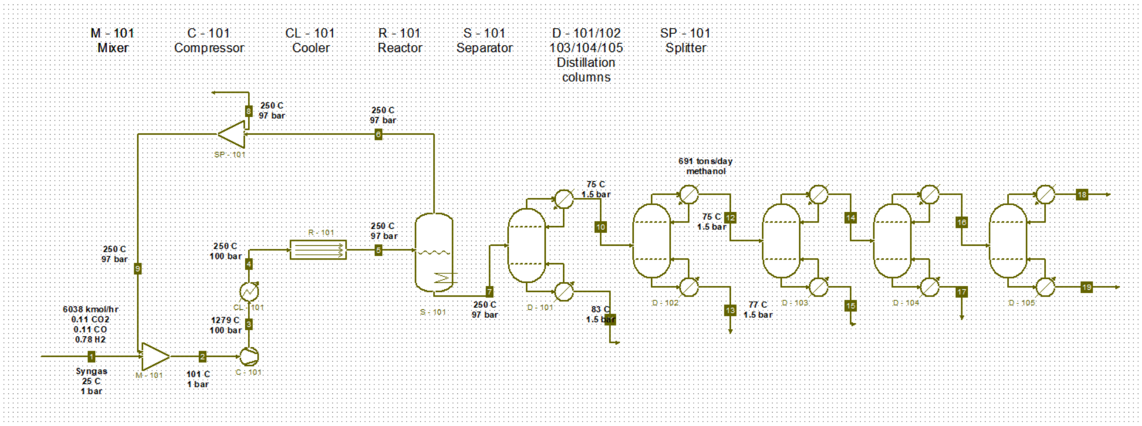


Figure 2.6.2. The Process Flow Diagram of methanol production with five distillation columns

Figure 2.6.2 demonstrates the process flow diagram of the methanol production with five distillation columns. The five distillation columns are used to purify the methanol from the compounds that occur as the result of some side reactions in the reactor. For report 2 the Aspen analysis focuses on the main reactions, therefore side reactions are not included in the mass balance calculations.

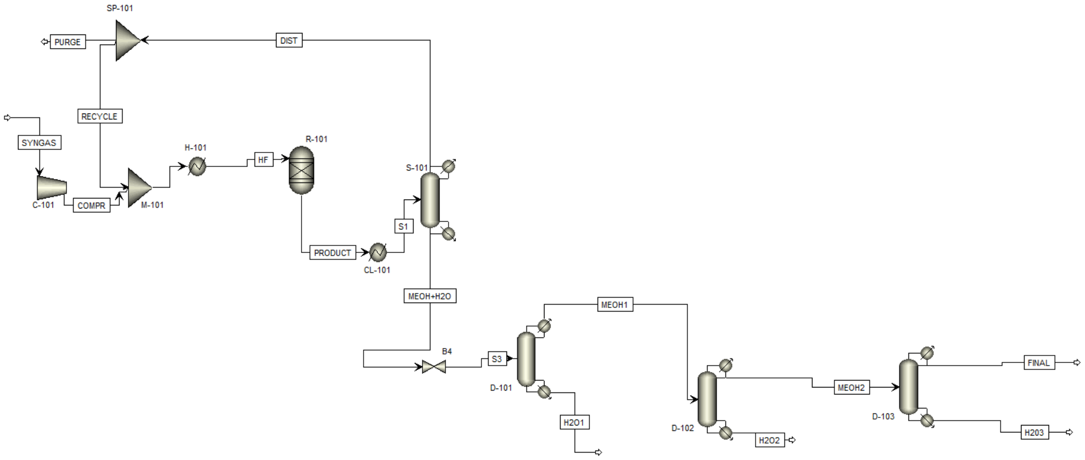


Figure 2.6.3. Aspen Plus Simulation of our PFD.

Description of processes involved in methanol production

Natural gas is usually used as the main raw material in large-scale production plants to produce synthesis gas, which is then needed for the synthesis of methanol. The optimization of synthesis gas for the production of methanol should be taken into account; however, a detailed explanation of the available technological routes (such as reforming the feedstock) used in the production of synthesis gas is not included in this report.

Pretreatment of syngas

Preparing or pretreating synthesis gas is the first stage in the production of methanol. Synthesis gas must be purified of contaminants prior to entering the process flow in order to meet the desired specification requirements (Cheng, 1994). For example, sulfur from synthesis gas (<0.1 ppm) in conventional methanol plants needs to be removed because it poses a risk to many active metals and can cause catalyst deactivation (Cheng, 1994).

Honeywell UOP currently owns the Selexol process, which was first created by Allied Chemical Corporation. It makes use of polyethylene glycol dimethyl ethers (DMPEG) using operating temperature range from 5 to 40 °C (Higman, 2011).Being able to function in this temperature range results in significantly lower expenses because refrigeration is not required. Compared to other gas purification techniques, it is a physically solvent-based process that runs at comparatively low temperatures. The high selectivity and versatility of the Selexol process in handling different gas streams are well known (Higman, 2011).

Production of methanol from syngas

The first and main step of the production process is the methanol synthesis from syngas, which consists of hydrogen, carbon monoxide, and carbon dioxide mixture. This process is a hydrogenation of carbon monoxide and carbon dioxide, which usually uses a Cu-based catalyst, usually mixed with ZnO on an Al_2O_3 support. The $Cu/ZnO/Al_2O_3$ catalysts used in industrial applications exhibit high efficiency and selectivity, approximately 99%. This is crucial due to the potential formation of undesired byproducts like methane, ethane, higher order alcohols, and others (Matzen, 2016).

The following is a process description for methanol synthesis using a catalyst $Cu/ZnO/Al_2O_3$ with 5% copper loading and a 1/1 ratio of zinc to copper at 250°C and 100 bar. The temperature and pressure conditions are taken by simulation test in the Aspen software where this combination demonstrated the biggest amount of methanol product rate. The Lurgi reactor (R-101) combines the functions of a reactor and a shell and tube heat exchanger. Boiling water serves as the cooling agent on the shell-side while the catalyst is packed within the tubes. This reactor design permits an almost isothermal operation (Cheng, 1994).

The stream 1 containing syngas with a 50 bar pressure and 50 °C temperature goes into the compressor (C - 101) where its pressure is raised to the 100 bars. In the compressor the temperature of the sample increases to 144 °C. Then the outer stream 2 of the compressor goes to the mixer (M - 101) to mix with recycle stream 9. After, it travels to the heater (H - 101), which is used to bring up the temperature till 250° C after the compressor. As the heating product water vapor is used at 360°C and 20 bars. Once required conditions are fulfilled, syngas enters a plug flow reactor (R-101). The reactor (R-101) operates at the mentioned pressure and temperatures and a heterogeneous catalyst is used.

Once the reactions take place the product goes through stream 5 to the cooling unit (CL - 101) that cools the synthesized product until 32°C in order to liquify the methanol. Cooling occurred in the heat exchanger with cold water. Cooled product goes to the separation unit (S - 101), where the sample is separated to the methanol and water solution and other gaseous compounds. Stream 6 is divided into stream 7 which goes as a recycle and stream 10 that is used to get the main product.

Methanol Purification

The separation process is vital in methanol production to achieve the necessary purity levels. Distillation is the primary method utilized in the methanol manufacturing process due to its effectiveness in isolating methanol from other components, yielding a desired purity of 99.85%. The advantage of distillation lies in exploiting methanol's lower boiling point (64.65°C) compared to other syngas components. This characteristic enables precise control over the separation process, facilitating the production of high-purity methanol.

First, stream 11 containing methanol and water goes into the first distillation column (D - 101) where the methanol produced in the separator performs a stripping action to separate the methanol liquid from the water. However, the first column does not give the purity of the 99.85% that is required. So the top product (stream 10) of first column (D - 101) is goes to second column (D - 102), where approximately 99.85% methanol product comes out overhead (stream 12).

In general, the methanol concentration in the bottom of the distillation columns is within the range of 0.01%-0.1% (Zhang et al., 2010). The distillation columns can not separate the methanol from water to the 100%.

The stream 6 shows the recycle stream which comes from the separator (S - 101). It delivers the not reacted syngas amount to the mixer (M - 101). The splitter (SP - 101) redistributes each of the components present to the feed stream.

III. Major equipment design

In this chapter 5 main equipment: the reactor, heat exchanger and three distillation columns are going to be designed. The design methods and working principles of each of them will be discussed as well.

3.1. Reactor design

The reactor is the central important component of any chemical plant. It may not always draw notice because of its size or appearance, but it plays a crucial role in functionality and influences the overall design. The production of methanol takes place via the Lurgi reactor, which uses a tubular fixed bed reactor under quasi-isothermal conditions and where a catalyst in tubes surrounded by boiling water. Recycled gas from the synthesis loop is combined with syngas generated in the reformer portion to feed the reactor.

3.1.1 Methanol reactor description

Temperature control is crucial since the synthesis reaction is substantially exothermic, making heat removal a crucial step (Tijm et al., 2001). A high heat flow results in fewer tubes, smaller furnaces, and hence lower costs (Aasberg-Petersen et al., n.d.). There are two main types of reactor technology that are widely employed in commercial settings:

1) multiple bed reactors
2) single bed converters

Multiple catalyst bed reactors regulate the reaction temperature by dividing the catalyst mass into multiple pieces and arranging cooling devices in between. Generally bed sizes are chosen to enable the reaction to reach equilibrium conditions. While the single bed reactors operate as effective heat exchangers because heat is continuously transferred from the reactor to a heat-removing medium. Today, the majority of commercial methanol production processes (such as gas-phase reactor technology and gas-solid-liquid technology) use a solid catalyst floating in a liquid medium to effectively extract heat from the reaction. As a result, it has a higher single-pass conversion and is easier to manage the reaction temperature than a standard solid reactor. The Lurgi reactor refers to the single bed (Tijm et al., 2001).

Reactor types that are used for catalytic processes include stirred tanks, bubble columns, two- and three-phase fluidized beds, moving beds, fixed beds, and trickling beds. Fixed-bed reactors are the most significant types of reactors used in catalyzed processes. The model reactor is the ideal plug flow reactor (PFR). Reagents enter tubular reactors continuously, and products exit when they are removed.

The vertical shell and tube heat exchanger with fixed tube sheets of the Lurgi Methanol Reactor has the appearance of a heat exchanger. There is an inert material bed under the catalyst in the tubes. The heat of reaction produces steam, which is removed below the upper tube sheet. Steam pressure control is used to obtain exact control over the reaction temperature. High yields at low recycle rates are possible while operating at isothermal conditions. Furthermore, there are as few byproducts as possible (Palma et al., 2018).

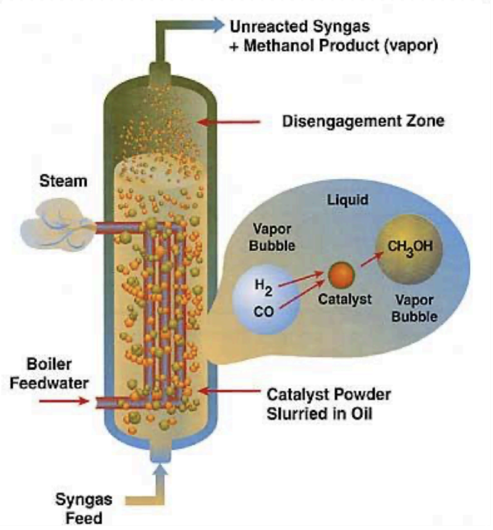


Figure 3.1.1. Design of Lurgi reaction (*Methanol Fuels*, n.d.)

Table 3.1.1 Tubular fixed single bed characteristics (Dieterich et al., 2020; Wu-Hsun Cheng (Editor), 1994)

Description	Water is boiling on the shell side of tubes that contain catalysts. The reactor operates as a trickle bed reactor.
Temperature limit	<270 °C, high temperatures lead to tube blocking due to the catalyst

	swelling
Temperature control	To prevent hotspot temperatures over the limit, the medium temperature must be lower; big temperature gradients in radial and axial direction
Temperature	250-270 °C
Pressure	50-100 bar

The operating conditions of converters affect the performance of the reactor and control the temperature profile throughout the reaction path and the amount of heat recovery. Table 3.1.2 summarizes reported exemplary operating parameters.

Table 3.1.2 The experimental operation conditions

Operating conditions	
Temperature (°C)	250 °C
Pressure (bar)	100 bar
Chosen catalyst	$CuO/ZnO/Al_2O_3$

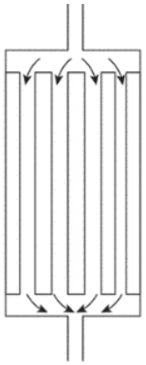


Figure 3.1.2. Design of the tubular reactor

Because of their huge light surface area, ease of fabrication, and capacity to scale up processes, tubular reactors are commonly accessible for applications used in Lurgi methanol production . By employing thin tubes with a maximum diameter of 10 cm and lighting the reactor from several angles, large surface areas can be achieved.

Table 3.1.3 shows the mass flow rate specification of the feed syngas which was taken from Aspen results. Further it will be used for the calculations of the volume of the reactor.

Table 3.1.3 Mole fraction of feed

Feed specification	**Mole fraction**
CO_2	0.11
CO	0.11
H_2	0.78

3.1.2. Design for the tubular reactor

The volume of the reactor is defined with the weight of th catalyst because the rate of the reaction is based on the catalyst weight. So the formula for the catalyst weight according to the (Fogler, 2016)

$$\frac{dX}{dW} = \frac{k(1-X)*(1-\alpha W)^{\frac{1}{2}}}{F_{A0}} \qquad (3.1.1)$$

where,

$X - conversion,$ %;

$\alpha - pressure\ drop,\ bar;$

$F_{A0} - flow\ rate,\ m^3/s$

$k - equilibrium\ constant;$

$W - weight\ of\ the\ catalyst,\ kg;$

Equation for the thermodynamic equilibrium constant to find the reaction rate constant (Wilkinson et al., 2016):

$$\beta_1^* = K_1^* \frac{p_{H_2O} * p_{CH_3OH}}{p_{CO_2} * p_{H_2}} \qquad (3.1.2)$$

$$\beta_2^* = K_2^* \frac{p_{H_2O} * p_{CO}}{p_{CO_2} * p_{H_2}} \qquad (3.1.3)$$

where,

$\beta_i^* - thermodynamic\ equilibrium\ constant;$

$K_i^* - thermodynamic\ constant;$

$p_i - partial\ pressure$

Equation for the rate constant:

$$k_i = A_{i,473} * exp\,[(\frac{E_a}{T_{base} * R}) * (1 - \frac{T_{base}}{T})] \quad (3.1.4)$$

where,

$k_i -$ $rate\ constant,\ s^{-1}$;

$A_{i,473} -$ $pre - exponential\ factor,\ s^{-1}$;

$E_a -$ $activation\ energy,\ kJ * mol^{-1}$;

$T_{base} -$ $base\ temperature,\ K$;

$T -$ $temperature,\ K$;

$R -$ $universal\ gas\ constant\ J * K^{-1} * mol^{-1}$.

Reaction rate constant is calculated in the excel file and equal to 0.026093716.

The conversion X is equal to 32.28%, pressure drop α=3, the flow rate from report 2. Then the Equation 3.1.1 is

$$\frac{dX}{1-X} = \frac{k*(1-\alpha W)^{\frac{1}{2}}}{F_{A0}} dW \quad (3.1.5)$$

Take integral of the Equation 3.1.5

$$ln(\frac{1}{1-X}) = \frac{k}{F_{A0}} * \frac{2}{3\alpha}[1 - (1 - \alpha W)^{\frac{3}{2}}]$$

$$ln(\frac{1}{1-0.3228}) = \frac{0.026093716}{6.859} * \frac{2}{3*3}[1 - (1 - 3W)^{\frac{3}{2}}]$$

W = 67.82 kg

Table 3.1.4. Catalyst volume calculation parameters

CO_2	
F_{A0} - inlet flow rate	24691.4 kg/hr 6.859 kg/s
X - required conversion of component A	32.28%
α- pressure drop	3 bar

k - reaction rate constant	0.026093716
W - weight of the catalyst	67.82 kg

Volume of the catalyst

$$V_c = \frac{W}{\rho} \quad (3.1.6)$$

V_c - volume of the catalyst, m^3

W - weight of catalyst, kg

ρ - density of the catalyst, kg/m^3

$V_c = \frac{W}{\rho} = \frac{67.82}{2000} = 0.03391\, m^3\, k = 33910\, cm^3$

Volume of the reactor :

$\frac{0.03391}{0.5(voidage)} = 0.06782\, m3$

0.11304 * 8000 tubes = $542.56\, m^3$

$\frac{L}{D}$ ratio = $\frac{976}{3}$ from Report 2

L - length, m

D - diameter, m

L = $\frac{976}{3}$* D

V= $\pi R^2 * L = \frac{\pi D^2}{4} * \frac{976}{3} * D$

D = 0.0510 m

L = 16.6 m

A quantity known as the reactor's space time can be defined as

$$\tau = \frac{V_t}{q_r} \quad (3.1.7)$$

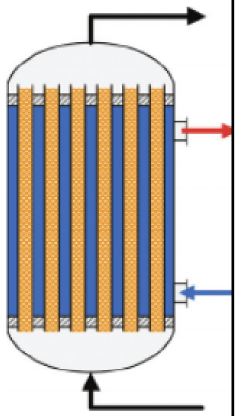
(Ravi, 2017)

Table 3.1.5. Calculation of the space time:

q_r is the volumetric flow rate . before reactor stream	10046.9 m^3/hr 2.791 m^3/s

V_t volume of the tubular reactor	542.56 m^3
τ space time	194.39 s

Table 3.1.6 Lurgi reactor design specifications

Specifications		
Volume of the reactor	542.56 m^3	
Diameter of one tube	0.0510 m	
Length of one tube	16.6 m	
Number of tubes	8000	
Catalyst Bed voidage	0.5	
Catalyst Particle density	2000 kg/cum	

3.2 Heat exchanger design

The heat exchanger plays a key role in optimizing the methanol production process, providing the necessary temperature conditions for a chemical reaction. In a specific task, the heat exchanger is used to heat syngas from a temperature of 140°C to 250°C using water vapor with a temperature of 360°C and a pressure of 20 bar. This makes it possible to improve the efficiency of the methanol synthesis reaction by increasing the rate and conversion of reagents. The heat exchanger is made in the form shell and tubular unit, where heat transfer occurs between water vapor in tubes and high pressure gas in the shell. These partitions allow heat to be transferred from the hotter steam to the colder synthesis, while preventing their direct contact. This method of heat transfer is efficient and safe, since it minimizes the risk of contamination of one stream by another.

An important part of the operation of the heat exchanger is the precise maintenance of the set syngas temperature, which is critical for the activity and durability of the catalysts used in the methanol synthesis process. Temperature control is carried out using automated control systems that regulate the flow of steam and its temperature depending on the current heat demand.

3.2.1.The working principle of heat exchanger

The heat exchanger is needed to heat up syngas before entering the reactor where the methanol is synthesized. The temperature of the stream after the mixer M-101 is equal to 142℃ and it have to be heated to 250 ℃. In order to achieve this temperature of the syngas, water vapor is used at 360 ℃ and 20 bars. Where, the hot stream is on the tube side and cold stream is on the shell side. Important information has been added to the table.

Table 3.2.1. Physical properties and conditions of syngas and water vapor.

Property	Tube Side		Shell side	
Phase	Vapour (Inlet)	Vapour (Outlet)	Vapour (Inlet)	Vapour (Outlet)
m, mass flow, kg/sec	17.51	17.51	11.2	11.2
	17.51		11.2	
T, temperature, ℃	142.8	250	360	254
C_p,Specific heat, J/kgK	2141	2141	3279	3295
	2141		3285	

According to the Aspen software of the whole plant the heat exchanged in the H-101 was Q = 3944kW. Also, the Aspen simulation of individual units was created. The heat duty of the unit was 4135kW, that is very close to the intended temperature. In addition, the heat duty was calculated manually in excel file.

The heat energy was calculated by the following equation (Towler & Sinnott, 2012b):

$$Q = m * c_p * \Delta T \tag{3.2.1}$$

Calculating the heat balance of the heat exchanger in the tube side:

$$Q = 11.2kg/sec * 3285J/kgK * (523K - 416K) = 3936kW \quad (3.2.2)$$

The area of the heat exchanger can be calculated using the heat generated above.

$$Q = A * U * \Delta T_m \quad (3.2.3)$$

It was calculated in the Appendix that the value of ΔT_m is 91.9 K.
U of the heat exchange was assumed as 250 $\frac{W}{m^2 °C}$ using the figure.
The are of the heat exchanger could be found by the formula below:

$$A = \frac{Q}{UT_m} = 171.5m^2 \quad (3.2.4)$$

3.2.2. Materials selection

It is essential to choose appropriate material for equipment design as it affects the durability and lifespan of the heat exchanger. Incorrect material can ruin installations and completely disable them in a short period of time, which will lead to great losses and loss of time. There are several main characteristics that should be considered during the material selection(Ashby, 2016):

1. Corrosion
2. Thermal and mechanical fatigue
3. High maintenance and replacement cost
4. Heat transfer efficiency

Taking into account the conditions above, there are several variants of the materials:

1. Stainless steel: Provides excellent corrosion resistance, especially in the presence of chlorides and other aggressive media that may be present in synthesis gas streams. It is able to withstand temperatures up to about 870°C, ensuring reliable operation at 200°C without any complications.

2. Carbon steel: Although carbon steel is economical, it often needs additional coatings or treatments to resist corrosion at high temperatures and pressures. As a rule, it is suitable for use at temperatures up to about 400°C. However, its suitability largely depends on the specific composition of the synthesis gas.
3. Nickel alloys: These alloys work exceptionally well in harsh environments. They are stable at high temperatures and pressures and provide excellent protection against corrosion and oxidation. If budget constraints allow, these materials are well suited for such difficult operating conditions.

   Finally stainless steel or carbon steel are recommended to use.(Perry & Green, 2008)

3.2.3. Equipment design

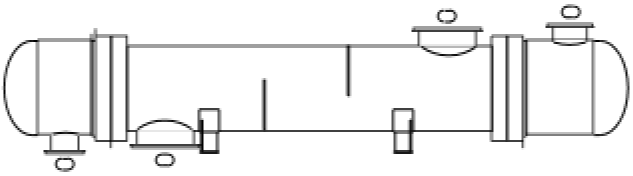


Figure 3.2.1. Schematic design of heat exchanger.

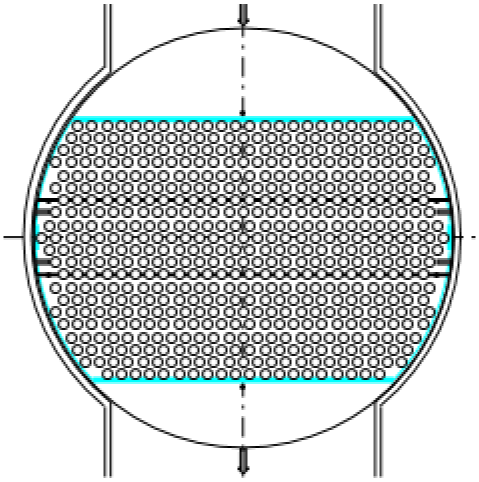


Figure 3.2.2. Tube layout of the exchanger.

3.3 Distillation columns design

3.3.1. Introduction to the distillation

Distillation - the crucial and final part of obtaining the necessary methanol product. The distillation is in the multistage rectification type, operated in batch or continuous mode. In the case of separating methanol, the process is continuous, as this mode allows for a steady feed into columns and continuous withdrawal of the products. For the large-scale industry, it is mandatory for the process to be undisrupted.

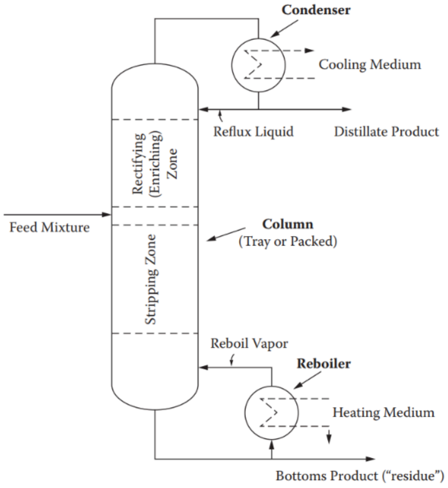


Figure 3.3.1. Basic distillation diagram

Figure 3.3.1 above shows the basic working principles and diagram of the continuous distillation unit. The distillation tower is usually fed with the mixture near the center, hence the stripping zone is located below the feed point, and rectifying zone above the feed point. Heat to the column is added by the vapor from the reboiler, and removed in a condenser to provide the distillate product. Some part of the distillate returns to the column as the reflux liquid (Lyle F. Albright, 2009).

The difference between the methodologies in the case of distillation is connected with the number of columns in the whole installation. The simplest scheme is the two-column distillation, shown on Figure 3.3.2 below (Lyle F. Albright, 2009).

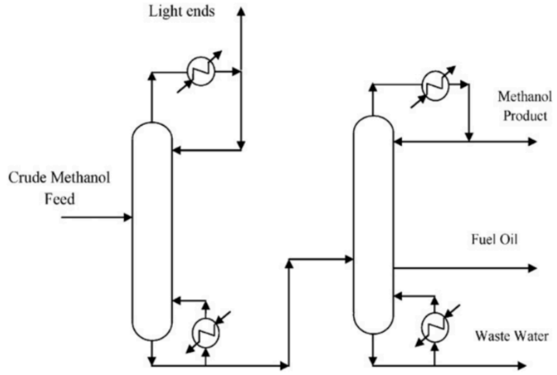


Fig. 1. Schematic diagram of the traditional two-column methanol distillation.

Figure 3.3.2. Two-column distillation

Before the product is suitable for commercial usage, water and other impurities found in crude methanol as extracted from the synthesis stage must be eliminated. Federal grade AA methanol is generated by two, three, and occasionally even four tower distillation systems, while fuel grade methanol can be produced with a single distillation tower. The by-products of the methanol synthesis catalyst, which include higher alcohols, paraffinic hydrocarbons, ethers, ketones, and aldehydes, determine how much distillation is needed. The synthesis catalyst's kind, age, and loop operation parameters all affect how much by-product is produced. Ethanol is the most troublesome contaminant.

Ethanol beyond 10 ppm is one of the more frequent issues with off-spec methanol, and the separation of ethanol from methanol is particularly challenging. A few trays down from the top of the refining column is where the product, methanol, is removed. Recirculating the column and separating any light ends that may have passed the topping column are done through the top of the column. Higher boiling alcohols are taken from the bottom of a few trays and are found further down the column. Fusel oil is the term used to describe this methanol stream that contains heavier hydrocarbons such paraffins and higher alcohols. Traditionally, the fusel oil has been burned in the utility boiler or primary reformer, or it has undergone additional processing to extract the methanol from the byproducts.

The refining column's bottom is cleared of water. To get rid of any organics, this water is usually subjected to some kind of biological treatment. The topping column bottoms in the three-column system go to an atmospheric refining column after passing through a pressurized refining column. Methanol of federal grade AA is removed near the top of both refining columns. The three-column approach can save the necessary distillation heat input by 30–40%, albeit being more expensive. To create U.S. federal grade AA methanol, most modern methods use either a two- or three-column distillation system, while occasionally a four-column system is employed. Generally speaking, multicolumn systems are only viable when energy costs are unreasonably high (*Separation Process Technology I*, n.d.)

3.3.2 Calculation of relative volatility

To calculate the saturation pressure of methanol and water needed to determine relative volatilities, Antoine's constants were used and put in the equation below.

$$log_{10}P = A - \frac{B}{C+T} \qquad (3.3.1)$$

where P is in kPa and T is in Celsius.

The saturated vapor pressure of methanol and water at different temperatures for each distillation column are provided below in Tables 3.3.1, 3.3.2, 3.3.3.

Table 3.3.1. The saturated vapor pressure (kPa) of methanol and water at feed, top and bottom temperatures for D-101 column.

	Methanol	Water
34.80 (feed)	27.6493	5.54727
73.47 (bottom)	142.378	36.0638
70.22 (top)	126.026	31.3844

Table 3.3.2. The saturated vapor pressure (kPa) of methanol and water at feed, top and bottom temperatures for D-102 column.

	Methanol	Water
70.22 (feed)	126.026	31.3844
73.02 (bottom)	140.014	35.3827
64.13 (top)	99.5693	23.9919

Table 3.3.3. The saturated vapor pressure (kPa) of methanol and water at feed, top and bottom temperatures for D-103 column.

	Methanol	Water
64.13 (feed)	99.5693	23.9919
69.87 (bottom)	124.362	30.9127
63.49 (top)	97.0806	23.3092

In order to determine the loss degree of materials throughout the methanol production process to estimate the quantity of methanol produced more precisely, we can compute the relative volatility of the liquid in the tower.

$$\alpha = \frac{P^{*}_{LK}}{P^{*}_{HK}} \tag{3.3.2}$$

Where, α - relative volatility of liquid in tower, P is saturation pressure. The average volatility α_{av}

$$\alpha_{ave=}\sqrt{\alpha_{top} \cdot \alpha_{bottom}} \tag{3.3.3}$$

For example, for D-101 column, the relative bottom and top volatilities are

$$\alpha_{bottom} = \frac{142.378}{36.0638} = 3.9479 \approx 3.95 \tag{3.3.4}$$

$$\alpha_{top} = \frac{126.026}{31.3844} = 4.0156 \approx 4.02 \tag{3.3.5}$$

Therefore, the average volatility for D-101 column is

$$\alpha ave = \sqrt{4.02 \cdot 3.95 = 3.98} \tag{3.3.6}$$

Calculations are shown in Excel. Further these values will be used to calculate the minimum number of theoretical plates. In Table 3.3.4, calculated average volatilities for each distillation column are provided.

Table 3.3.4. The calculated average volatilities for each distillation column.

Distillation Columns	α_{ave}
D-101	3.98
D-102	4.05
D-103	4.09

3.3.3 Minimum number of theoretical plates (trays): Fenske Equation

The equation for determining the minimal number of trays needed for multicomponent distillation at total reflux was initially derived by Fenske in 1932. The stages were assumed to be equilibrium stages for the derivation. As illustrated in Figure 3.3.3, consider a multicomponent distillation column functioning at total reflux (*Separation Process Technology I*, n.d.) .

$$N_{min} = \frac{ln(\frac{x_D}{1-x_D} \cdot \frac{1-x_B}{x_B})}{ln(\alpha_{ave})} \tag{3.3.7}$$

where, x_D- mole fraction of methanol in top product, x_B - mole fraction of water in bottom product, α -average volatility, and N_{min} - minimum number of theoretical stages. As the result of the calculations, the N_{min} = was obtained.

$$N_{min} = \frac{ln(\frac{0.91_D}{1-0.91} \cdot \frac{1-0.59}{0.59})}{ln(3.98)} = 1.38 \tag{3.3.8}$$

Calculations are shown in Excel. In Table 3.3.5, calculated Minimum number of theoretical plates for each distillation column are provided.

Table 3.3.5. The calculated minimum number of theoretical plates for each distillation column.

Distillation Columns	N_{min}
D-101	1.38
D-102	3.48
D-103	6.57

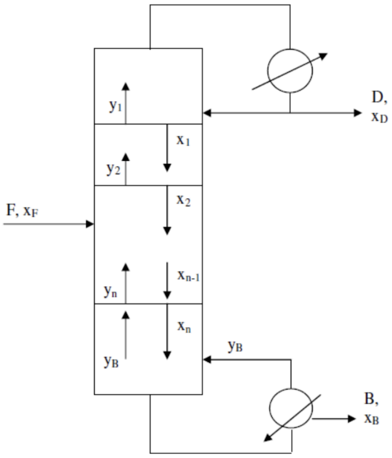


Figure 3.3.3. Multicomponent column at minimum trays

Plotting the Mc-Cabe Thiele diagram shows the same results, from the diagram it is seen that the minimum number of theoretical stages is 2.

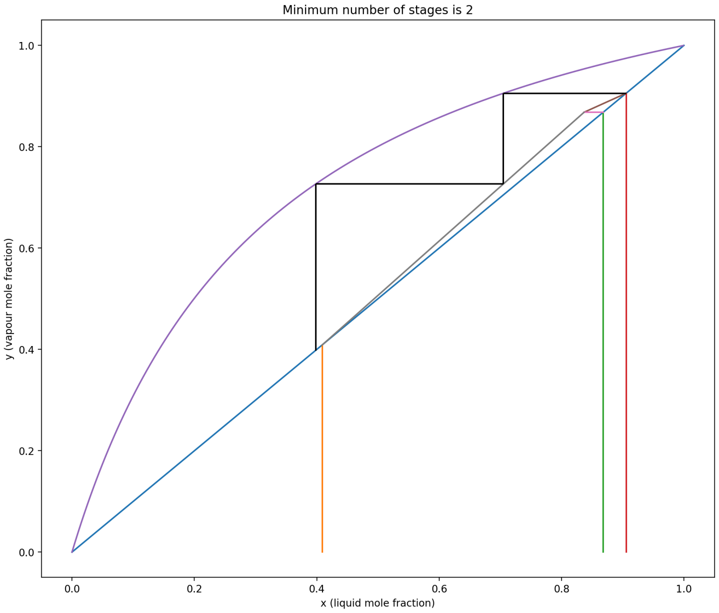


Figure 3.3.4. Mc-Cabe-Thiele diagram for the Column №1

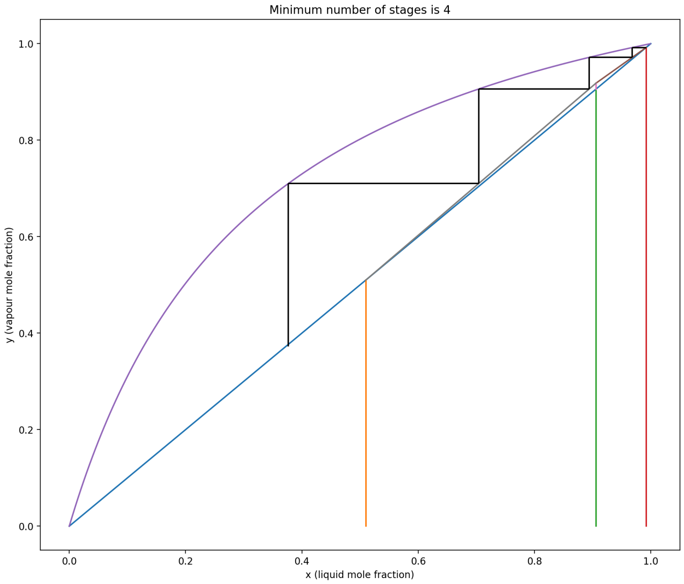


Figure 3.3.5. Mc-Cabe-Thiele diagram for the Column №2

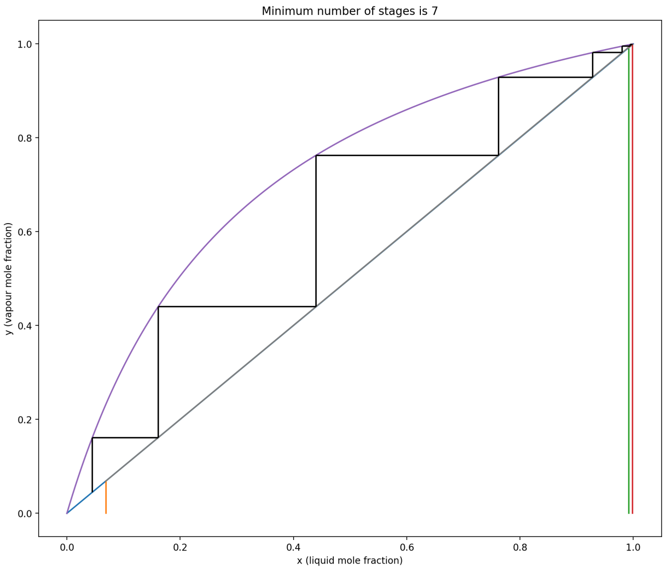


Figure 3.3.6. Mc-Cabe-Thiele diagram for the Column №3

3.3.4 Minimum Reflux ratio: Underwood Equation

In multi-component systems, there are distinct pressure points in the stripping and rectifying sections if one or more of the components are present in only one of the products. Underwood created a different analysis in this instance to determine the minimum reflux ratio (Wankat, 1988). When non-distributing light non-keys are present, a pinch point will occur in the stripping section; nevertheless, the presence of non-distributing heavy non-keys causes a pinch point of constant composition at minimum reflux in the rectifying section.

In a rectification, the most crucial operational variable is the reflux ratio R = L/D; the operating pressure and feed condition are fixed. Between the lowest reflux ratio Rmin and infinite R = ∞, R might change. The reflux ratio in a column with an infinite number of stages in the rectification and stripping sections that still permits separation is known as the minimal reflux ratio, or Rmin. By considering a constant relative volatility alpha, the minimum reflux ratio may be computed using Underwood's correlation. Both of the Underwood correlations can be combined for a binary mixture (*Separation Process Technology I*, n.d.).

$$R_{min} = \frac{1}{\alpha - 1}\left[\frac{x_D}{x_F} - \alpha \cdot \frac{1 - x_D}{1 - x_F}\right] \tag{3.3.9}$$

$$R_{min} = \frac{1}{3.98-1}\left[\frac{0.91}{0.59} - 3.98\cdot\frac{1-0.91}{1-0.59}\right] = 0.21 \qquad (3.3.10)$$

Where:

α - constant relative volatility,

x_F - mole fraction of water in bottom product,

x_D -mole fraction of methanol in top product,

R_{min} - minimum reflux ratio.

The results of the calculations for 3 distillation columns were shown below in Table 3.3.6. The calculation steps are provided in Excel.

Table 3.3.6. The calculated minimum reflux ratio values for each distillation column.

Distillation Columns	R_{min}
D-101	0.21
D-102	0.65
D-103	4.69

3.3.5 Theoretical number of stages: Gilliland Correlation (*Separation Process Technology I*, n.d.)

The following calculations are for the D-101 distillation column. Further calculations are done in the Excel file.

The effective reflux ratio is chosen 0.6 times higher than the minimum.

$$R = R_{min}*0.6 = 1.2$$

Gilliland provides a diagram that illustrates the relationship between the reflux ratio, the minimal reflux ratio, the theoretical number of stages, and the reflux ratio. The x-coordinate is

$$\left(\frac{R-R_{min}}{R+1}\right) = \frac{1.2-0.21}{1.2+1} = 0.45$$

From the Figure 3.3.7, below, the value of the ordinate can be seen

$$\left(\frac{N-N_{min}}{N+1}\right) = 0.3$$

With the N_{min} = 1.38 value obtained previously, the required theoretical number of stages including the reboiler is calculated

$$N = (\frac{0.3+N_{min}}{1-0.3}) = \frac{0.3+1.38}{1-0.3} = 2.4$$

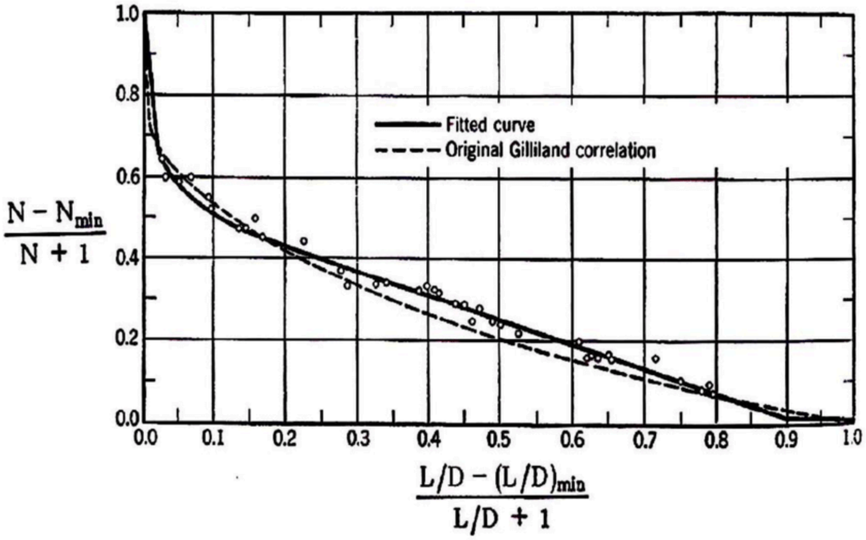


Figure 3.3.7. Gilliland correlation as modified by Liddle (1968) (*Figure*, n.d.).

Table 3.3.7. The calculated number of stages for each distillation column.

Distillation Columns	N
D-101	2.4
D-102	3.97
D-103	10.64

3.2.6. Tray analysis and hydraulic plots

Tray analysis and hydraulic plots play a vital role in optimizing distillation column performance. Tray analysis involves assessing the efficiency and effectiveness of each tray in the column. Various parameters, such as the number of holes, cross-sectional area, and tray spacing, are evaluated to achieve the most efficient distillation process.

Hydraulic plots, in contrast, offer a visual depiction of fluid flow patterns, illustrating the distribution of both liquid and vapor across the trays. The plots are useful for identifying potential issues such as flooding or weeping, which can then be addressed by making adjustments to tray design or operating conditions. This ultimately improves the overall efficiency of the column. For a more comprehensive understanding of the distillation column analyses, all of the necessary data was attached to the appendix provided. Additionally, hydraulic reports from the Aspen Plus Software were attached with the report.

3.2.7. Column 1

Table 3.3.8. Column 1 specification sheet.

<table>
<tr><td colspan="4">Unit: Column 1</td></tr>
<tr><td colspan="4">Designation: Distillation column</td></tr>
<tr><td colspan="2">Feed flow rate (kmol h^{-1})</td><td colspan="2">1279.200</td></tr>
<tr><td colspan="2">Inlet temperature (℃)</td><td colspan="2">34.804</td></tr>
<tr><td colspan="2">Inlet pressure (bar)</td><td colspan="2">1.200</td></tr>
<tr><td colspan="2">Distillate flow rate (kmol h^{-1})</td><td colspan="2">6.396</td></tr>
<tr><td colspan="2">Bottom flow rate (kmol h^{-1})</td><td colspan="2">1272.800</td></tr>
<tr><td colspan="2">Condenser operating conditions</td><td colspan="2">Reboiler operating conditions</td></tr>
<tr><td>Condenser type</td><td>Total</td><td>Reboiler type</td><td>Kettle</td></tr>
<tr><td>Reflux rate (kmol h^{-1})</td><td>28.783</td><td>Boilup rate (kmol h^{-1})</td><td>176.413</td></tr>
<tr><td>Condenser temperature (℃)</td><td>68.068</td><td>Reboiler temperature (℃)</td><td>69.843</td></tr>
<tr><td colspan="4">Parameters of Column 1</td></tr>
</table>

Column diameter section-1 (m)	0.387
Column diameter section-2 (m)	1.044
Column height total (m)	6.096
Column height section-1 (m)	1.219
Column height section-2 (m)	4.877
Tray type	Sieve
Tray spacing (m)	0.6096
Construction material	Stainless steel
Distillate-to-feed ratio	0.005
Number of stages	12
Feed stage (above the stage)	4

3.2.8. Column 2

Table 3.3.9. Column 2 specification sheet.

Unit: Column 2	
Designation: Distillation column	
Feed flow rate (kmol h^{-1})	1272.830
Inlet temperature (℃)	69.843
Inlet pressure (bar)	1.200
Distillate flow rate (kmol h^{-1})	1186.277

<table>
<tr><td colspan="2">Bottom flow rate (kmol h^{-1})</td><td colspan="2">86.552</td></tr>
<tr><td colspan="2">Condenser operating conditions</td><td colspan="2">Reboiler operating conditions</td></tr>
<tr><td>Condenser type</td><td>Total</td><td>Reboiler type</td><td>Kettle</td></tr>
<tr><td>Reflux rate (kmol h^{-1})</td><td>5931.388</td><td>Boilup rate (kmol h^{-1})</td><td>7155.488</td></tr>
<tr><td>Condenser temperature (℃)</td><td>69.552</td><td>Reboiler temperature (℃)</td><td>67.225</td></tr>
<tr><td colspan="4">Parameters of Column 2</td></tr>
<tr><td colspan="2">Column diameter section-1 (m)</td><td colspan="2">6.012</td></tr>
<tr><td colspan="2">Column diameter section-2 (m)</td><td colspan="2">6.235</td></tr>
<tr><td colspan="2">Column height total (m)</td><td colspan="2">23.165</td></tr>
<tr><td colspan="2">Column height section-1 (m)</td><td colspan="2">20.117</td></tr>
<tr><td colspan="2">Column height section-2 (m)</td><td colspan="2">3.048</td></tr>
<tr><td colspan="2">Tray type</td><td colspan="2">Sieve</td></tr>
<tr><td colspan="2">Tray spacing (m)</td><td colspan="2">0.6096</td></tr>
<tr><td colspan="2">Construction material</td><td colspan="2">Stainless steel</td></tr>
<tr><td colspan="2">Distillate-to-feed ratio</td><td colspan="2">0.932</td></tr>
<tr><td colspan="2">Number of stages</td><td colspan="2">40</td></tr>
<tr><td colspan="2">Feed stage (above the stage)</td><td colspan="2">35</td></tr>
</table>

3.2.9. Column 3

Table 3.3.10. Column 3 specification sheet.

<table>
<tr><td colspan="4">Unit: Column 3</td></tr>
<tr><td colspan="4">Designation: Distillation column</td></tr>
<tr><td colspan="2">Feed flow rate (kmol h^{-1})</td><td colspan="2">1186.277</td></tr>
<tr><td colspan="2">Inlet temperature (℃)</td><td colspan="2">69.552</td></tr>
<tr><td colspan="2">Inlet pressure (bar)</td><td colspan="2">1.200</td></tr>
<tr><td colspan="2">Distillate flow rate (kmol h^{-1})</td><td colspan="2">1174.415</td></tr>
<tr><td colspan="2">Bottom flow rate (kmol h^{-1})</td><td colspan="2">11.863</td></tr>
<tr><td colspan="2">Condenser operating conditions</td><td colspan="2">Reboiler operating conditions</td></tr>
<tr><td>Condenser type</td><td>Total</td><td>Reboiler type</td><td>Kettle</td></tr>
<tr><td>Reflux rate (kmol h^{-1})</td><td>5872.075</td><td>Boilup rate (kmol h^{-1})</td><td>5840.617</td></tr>
<tr><td>Condenser temperature (℃)</td><td>69.536</td><td>Reboiler temperature (℃)</td><td>71.472</td></tr>
<tr><td colspan="4">Parameters of Column 3</td></tr>
<tr><td colspan="2">Column diameter section-1 (m)</td><td colspan="2">5.982</td></tr>
<tr><td colspan="2">Column diameter section -2 (m)</td><td colspan="2">5.494</td></tr>
<tr><td colspan="2">Column height total (m)</td><td colspan="2">20.117</td></tr>
<tr><td colspan="2">Column height section-1 (m)</td><td colspan="2">13.4112</td></tr>
<tr><td colspan="2">Column height section-2 (m)</td><td colspan="2">6.7056</td></tr>
</table>

Tray type	Sieve
Tray spacing (m)	0.6096
Construction material	Stainless steel
Distillate-to-feed ratio	0.99
Number of stages	35
Feed stage (above the stage)	24

IV. Minor equipment design

This chapter will cover the design and specifications of minor equipment.

4.1.Separator design

4.1.1 Vapor-Liquid Flash Separation

Vapor-liquid separators are employed in our process to separate two-phase inlet streams into pure vapor and pure liquid phases. This separation enhances product purity, especially when there's a notable volatility difference between components. In our case, the goal is to extract methanol and water from the unreacted syngas, where methanol content is typically low (3-6%).[was not used] Stream that comes out of the reactor is first cooled in the cooler till required temperature is reached and only then headed to the flash drum.

Two primary types of flash separators are available, depicted in Figure 4.1.1. The choice between them hinges on calculating the length-to-diameter (L/D) ratio. A vertical separator is recommended for L/D ratios between 3 and 5, while a horizontal separator is preferable for L/D ratios exceeding 5. This selection ensures efficient separation tailored to our system's requirements (Bahadori, 2014)

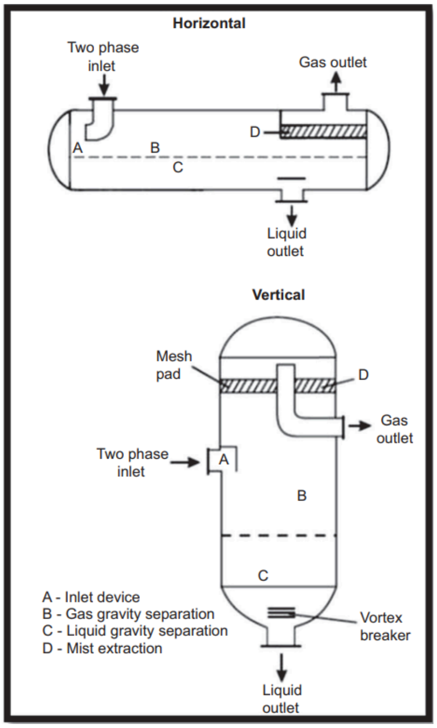


Figure 4.1.1. Types of flash separators (Bahadori, 2014).

The significant parameters for this separator to be calculated are only its length and diameter. The equations from the Appendix X will be used to determine the values and find the L/D ratio. (All calculations are presented in the Flash_calculations.xlsx file in the ESI)

Table 4.1.1. Design specifications of flash separator.

Vertical flash separator designs	**S-101**
Temperature (°C)	32
Pressure (bar)	100
Diameter (m)	1.95
Length (m)	6.05
Inlet Mass flow rate (kg hr^{-1})	117065.7

Overhead Mass flow rate (kg hr^{-1})	69862.3
Bottom Mass flow rate (kg hr^{-1})	47203.6
L/D ratio	3.10

L/D ratio turned out to be 3.10, which means our flash separator is vertical.

4.2.Mixer and splitter design

Gas mixing at the outset of the flowsheet plays a crucial role in blending the flow of unreacted gasses, pressurized to 100 bars, with the original syngas that has undergone compression to the same pressure level. Usually the mixing process takes place within the piping system,“T”- piece or “Y”-piece junctions can be used to connect the two inlet and outlet gas streams and perform mixing. The main point is to promote turbulence by adding Once the gas is homogeneously mixed, it enters the heater, where the combined gasses undergo heating to elevate their temperature up to 250℃. This preheating step is integral to priming the gasses for subsequent reactions or processes downstream in the system.

Within the Process Flow Diagram for our project, the splitter serves as a significant component within the recycle path, positioned adjacent to the vapor stream of the flash separator. Here, the purge stream is generated, which comprises both inserts and unreacted components, separated from the main stream at a ratio of 0.7. This purge stream is essential for maintaining the inerts within specified limits, ensuring the efficiency and stability of the overall process.

4.3.Compressors design

Compressor design was made by the manual (Compressors).

Table 4.3.1. Conditions for compressors

Equipment	**C-101**
Gas type	Syngas
Suction pressure (bar)	50

Discharge pressure (bar)	100
Specific Heat Ratio (J/kg K)	399 [36]
Suction temperature (K)	323.15
Volumetric flow rate (m^3 h^{-1})	2303.41
Mass flow rate, (kg h^{-1})	39,877.4

Compression ratio should be found in order to determine compressor stages. R values formula is:

$$R = \frac{P_d}{P_s} \qquad (4.3.1)$$

Where:

P_d - Discharge pressure

P_s - Suction pressure

After the calculation, the R value is 2 for C-101. Hence, the compressor is single stage.

Next step is to find the suction temprature.

$$T_d = T_s R^{(n-1)/n} \qquad (4.3.2)$$

By calculation the suction temperature is 645.17 K .

Volumetric efficiency and piston displacement also needs to be found using formula below:

$$VE\% = 93 - R - 8(R^{1/n} - 1) \qquad (4.3.3)$$

$$PD = \frac{ICFM}{VE} \qquad (4.3.4)$$

Finally, the volumetric efficiency and piston displacement is 90.98% and 1727.8 CFM.

Piston displacement (PD) reflects the capacity of a compressor, influenced by the dimensions, quantity, and kind of cylinders, as well as the revolutions per minute (RPM) of the compressor. The needed piston displacement (PD) user computed value essential for determining the appropriate size of a compressor necessary to manage the designated capacity. V is volumetric flow rate. So, PD equals 1727.8 CFM. ICFM is equals to 1571.96.

Determining the power required for every compressor is the final step. Each value was computed and displayed in Table 4.3.2.. All of these data will be used to select the compressor.

$$BHP = 0.00528 * \frac{n}{n-1} * P_s * PD * (R^{\frac{n-1}{n}} - 1) \tag{4.3.5}$$

Table 4.3.2. Conditions for compressors.

Equipment	**C-101**
R value	2
Discharge temperature (K)	645.17
Volumetric efficiency (%)	90.98
Piston displacement	1727.8 CFM
Power (kW)	4928.5

4.4. Cooler design

To characterize the heater and cooler, their heat duties were calculated. The heater is used to increase the temperature of the inlet stream that comes from pipelines, where recycle and syngas streams were mixed and headed into the reactor from about 142.8℃ to required 250℃. The cooler is used to condense the crude methanol and separate it from the unreacted gasses before they enter the flash drum. It cools the outlet stream from 250℃ to 32℃.

Calculations of heat duty values were done based on the values obtained from Aspen Plus V14 data analysis and then compared with the actual simulation results. Equation below was used to obtain the heat duties.

$$Q = m\, C_p\, \Delta T \tag{4.4.1}$$

Table 4.4.1 The final calculated values of cooler design.

Property	**Tube Side**		**Shell side**	
Phase	Vapour (Inlet)	Vapour liquid mixture (Outlet)	Liquid(Inlet)	Vapour liquid mixture (Outlet)
m, mass flow, kg/sec	8.6	8.6	6	3
	8.6		4.5	
T, temperature, ℃	250	32	15	102
C_p,Specific heat, J/kgK	20645	3727	4826	4871
	12186		4848	

According to Aspen simulation:

Area of cooler is 184 m^2. Q is equal to 9846 kW.

V. Plant location and Layout

5.1. Plant location criteria

Plant location is crucial, as it is highly influential on the plant economics, production rate, and environmental effect. Considering all of the important factors and variables, the Atyrau region was chosen as the plant location. Following criteria were used to justify the selection:

1. The raw material (syngas) should be available near the forecasted location;
2. Infrastructure level in the region of the chemical plant, including transportation networks, roads, or ports, should be on the highest level;
3. Market access should be advantageous, both for the export and import of the methanol after the production.

For choosing the plant location, the Special Economic Zones regulated by the government were the first priority. The main reason for that is companies in SEZs are exempted from corporate income tax, value added tax, and custom duties (*Invest in Kazakhstan | Special Economic Zones*, n.d.). The chosen SEZ is "National Industrial Petrochemical Technopark", which has the following tariffs:

Table 5.1.1 "NIPT" Special economic Zone's tariffs (*Invest in Kazakhstan | Special Economic Zones*, n.d.).

Tariff	**Cost (KZT)**
Water supply cubic meters (m^3)	333.334
Heat supply ($Gcal$)	19.5915
Power supply (kW)	19.152
Sewerage ($\frac{m^3}{hour}$)	169.064

Location factor is chosen to be 1.53, as Atyrau region is closely located to the major industrial cities of Russia, within the 1000 km range necessary for adjusting the location factor for another 10%.

5.1.1. Raw material availability

Almost 98% of all of the gas resources in Kazakhstan are located in the western part of the country, and 34.5% of all of the reserves are located in the Kashagan gas field and 17.3% in the Tengiz gas field, in the Atyrau region. NCOC is the company which has established the production in this field (*Natural Gas Industry of Kazakhstan: Key Features and Future Prospects*, n.d.). As the forecasted methanol plant will be located near the Kashagan gas field, purchasing the feedstock will be much cheaper. Additionally, the nearest gas field located in Russia is the Astrakhan gas plant, which produces 8340 metric tons of gas condensate per day (XM, 2021). Although it will be favorable to choose the gas field in Kazakhstan, due to lower prices and transportation convenience, the availability of such an option is economically favorable

5.1.2. Infrastructure development in the plant location region and market access

Transportation is the key factor in optimizing the plant economics, because locating the plant in the region without the well-established gas transportation network and supply chain could result in the additional expenses or even the absence of profitability. However, the Atyrau region has well-developed infrastructure, including the gas transportation network, crucial for acquiring raw materials.

Figure 5.1.1. Gas transportation networks in Kazakhstan

"Intergas Central Asia" is the major company in the field of transportation and maintenance of the gas pipelines ("KAZAKHSTAN'S OIL AND GAS INDUSTRY REVIEW," 2022). From Figure 5.1.1 it could be seen that there is a connection between Karachaganak gas pipelines with major cities of the region, like Atyrau, Uralsk, Samara, Astrakhan, and Orenburg.

The availability of many transportation corridors in the Atyrau region is another important factor contributing to the selection. First of all, there are already three major transportation roads, connecting the major city of the region, Atyrau, with Aktobe, Uralsk, and Astrakhan. Methanol is mostly transported by trucks, rails or sea shipping, and for the first case, locating the methanol plant along the road is crucial, so it will be possible to transport methanol drums for export and domestic use.

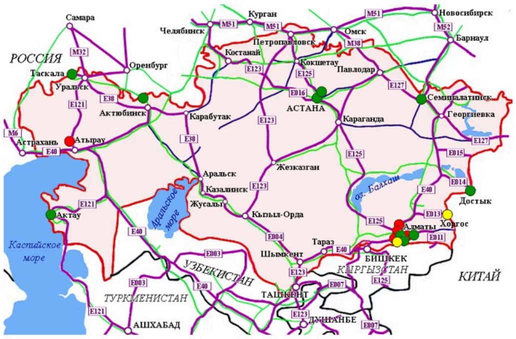


Figure 5.1.2. Transportation corridors in Kazakhstan (purple - existing, green - under construction)

For the railroad networks, methanol drums could be distributed first to the Aktobe region, then transported by railroad to the other regions. As for sea transportation, the option is to transport the cargo to the coastline ports, so it could be then exported to other countries by the Caspian Sea. However, this method is only relevant if some countries of the Caspian Sea region are interested in importing the Kazakhstani methanol.

Figure 5.1.3. Railroad networks of Kazakhstan

To sum up the transportation networks for all of the methods, it is clearly seen that the current location gives pleasant conditions for accessing both foreign and domestic markets, Land roads connect all of the major cities in the region, railroads and sea transportation are also available as alternative routes.

5.2. Plant Layout

A well-thought-out layout of the installation is an essential component of the design of the technological process, which significantly affects the efficiency of the technological unit and the overall economy of the enterprise. Key factors influencing the layout of the installation include: (1) economic factors such as operating and construction costs; (2) ease of operation and maintenance; (3) safety considerations; and (4) ensuring future expansion.

Economic factors

The operating units must be positioned as close to one another as feasible to reduce the expense of piping between pieces of equipment in order to create a more economically efficient plant.

Convenience of operation and maintenance

If an operation unit requires frequent operator monitoring, it is imperative to select a strategic location for the control room. It is important to arrange valves and instruments so that operators can easily access them. Sufficient workspace and headroom are essential for enabling effortless equipment accessibility. Furthermore, enough room needs to be set out for maintenance and future equipment replacement. In order to reduce the amount of time required for staff and vehicles to move between various process areas, it is also important to plan roadways and walkways (Towler & Sinnott, 2021).

Safety

Plant areas that pose a risk should be situated further away from office spaces and administrative buildings. Clearly marking emergency routes is also necessary in case of an accident. The leakage of syngas can cause difficulties in the respiratory tract. Also, most of the processes in the plant take place under high pressure and the gas is flammable .Thus, in order to carry out this processes, it is necessary to allocate a certain region located at a great distance from other facilities intended for the production of methanol and purification.

Future expansion

Future expansions should be considered when designing the layout of the plant. Glucose, the primary raw material used in the environmentally friendly and carbohydrate-based synthesis of THF, is now sourced from different glucose-producing companies. Nevertheless, cellulose, biowaste, vegetables, and other biomaterials can also provide sources of carbohydrates. As a result, future plans call for the construction of process units for the manufacturing of carbohydrates. When designing the plant layout in the beginning, this possibility should be carefully taken into account (Snow, 2002).

Plant Layout design

The main plant equipment are located in the Plant area 1 and Plant area 2 as the production of the methanol consist of the methanol synthesis and purification processes.

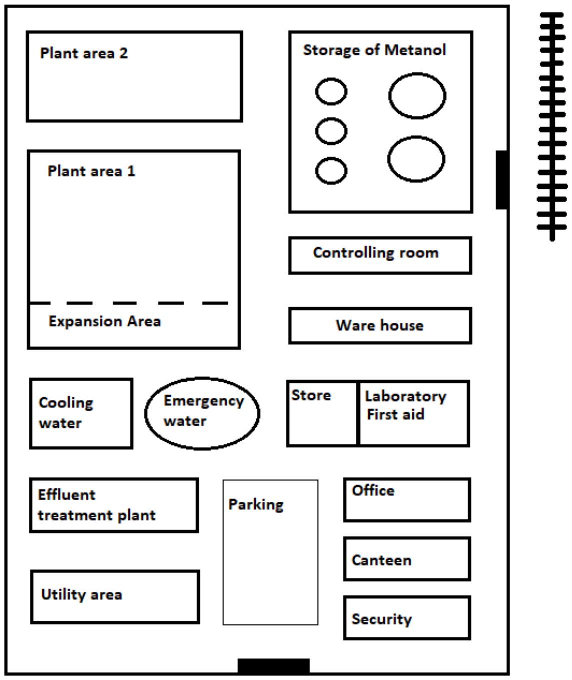


Figure 5.2.1. Methanol plant layout

The process sections occupy a significant part of the installation. The storage tanks for raw materials are ideally located next to the railway tracks and the territory of the plant. Since cooling is required for the main reaction, the cooling water supply systems are located next to the process area. For a quick response in case of an emergency, a fire station equipped with emergency water supply is located next to the enterprise. The laboratory and first aid are located almost in the middle of the plant. The control unit is conveniently located next to the storage facilities at a safe distance from the technological zones. The administrative office, the canteen and the security service are located in buildings where ordinary employees are housed, and are located separately from the production areas. There are two exits at the facility: one for staff and parking, and the other for transporting materials.

VI. Environment and waste streams

6.1. Environment

Methanol, also known as methyl alcohol and wood alcohol, is a light, colorless, extremely flammable liquid with a somewhat sweeter odor than ethanol. Because it has become an important additive in many regularly used items, everyone is exposed to tiny quantities of methanol every day. Methanol is a crucial component of biofuels generated from fats and oils because it functions as a catalyst in the manufacture of biodiesel fuel. Direct intake of more than 10mL can result in irreversible blindness due to destruction of the optic nerve, coma, central nervous system toxicity and perhaps death. These risks apply if methanol fumes are breathed (*Methanol Safety Tips from MSDS Experts*, 2014). In this chapter, the health and safety analysis of methanol, and other components will be considered.

6.1.1. Methanol Health Effects

According to the harmonized classification and labeling (CLP00) approved by the European Union, this substance is toxic if consumed, is toxic in contact with skin, is toxic if inhaled, causes damage to organs and is a highly burnable liquid and vapor. In addition, this substance is suspected of causing cancer, which is revealed by the classification provided by companies to ECHA in REACH registrations (*Methanol*, n.d.). Therefore, intoxication symptoms are irritation of eyes, skin, upper respiratory system; headache, drowsiness, dizziness, nausea, vomiting; visual disturbance, optic nerve damage (blindness); dermatitis (*Methyl Alcohol*, 2019).

100-250 mL can be deadly or cause blindness. The primary physiological impact of methanol oxidation to formic acid is acidosis. Methanol cannot pose a significant toxicity risk when handled in well-ventilated locations, and the NFPA (National Fire Protection Association) rates it as a minor health concern. The threshold limit value (TLV) for the American Conference of Industrial Hygienists (ACGIH) and the Occupational Safety and Health Administration (OSHA) is 200 ppm, with a short-term exposure limit (STEL) of 250 ppm and a limit that is instantly threatening to life and health of 25,000 ppm (English et al., 2015). The personal protection advice was given in Table 6.1.1.

Table 6.1.1 Personal sanitation and First aid information in case of poisoning with methanol (*Methyl Alcohol*, 2019).

Personal protection/sanitation	**First aid**
Skin: Prevent skin contact	**Eye:**Irrigate immediately
Eyes: Prevent eye contact	**Skin:**Water flush promptly
Wash skin: When contaminated	**Breathing:**Respiratory support

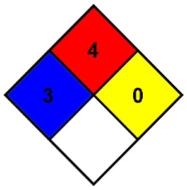
Remove: When wet (flammable)	**Swallow:** Medical attention immediately
Change: No recommendation	

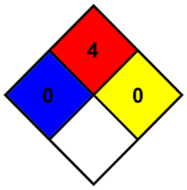
Methanol can be released to the environment from industrial use, such as producing of the substance, as an intermediate step in additional manufacturing of another substance, in processing aids at industrial areas, as processing aid and formulation of mixtures (*Methanol*, n.d.).

6.1.2. Health Effects of the main reactants

Among all of the reactants, it can be seen from Table 6.1.2 that all of the reactants are gasses under pressure. Hydrogen and carbon monoxide are flammable and carbon monoxide is the hazardous reactant. The sign "SA" in carbon dioxide NFPA diagram means that it is simple asphyxiant (Figure D2 in Appendix D), gas or vapor that can lead to unconsciousness or death by suffocation (asphyxiation). Explanations of NFPA diamonds and Hazard labellings are given in the Appendix D.

Table 6.1.2 ECHA hazard labels NFPA Ratings of reactants.

Component	Hazard classification & labelling	Hazard name	NFPA Hazard Diamond	Hazard	Value
Carbon monoxide (*Carbon Monoxide Safety Data Sheet P-4576*, n.d.)		Flammable		Health hazard	3
		Gas Cylinder		Flammability	4
		Health Hazard		Reactivity	0
		Acute			

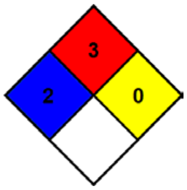
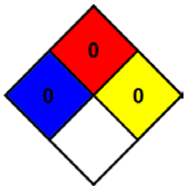
		Toxic			
Carbon dioxide (*Carbon Dioxide Safety Data Sheet P-4574*, n.d.)		Gas Cylinder		Health hazard	3
				Flammability	0
				Reactivity	0
Hydrogen (*Hydrogen, Compressed Safety Data Sheet P-4604*, n.d.)	 	Flammable		Health hazard	0
		Gas Cylinder		Flammability	4
				Reactivity	0

6.1.3. Health Effects of the main products

Water has no hazard and methanol is combustible, causes health hazards and is severely toxic according to Table 6.1.3.

Table 6.1.3. ECHA hazard labels NFPA Ratings of products.

Component	Hazard classification & labelling	Hazard name	NFPA Hazard Diamond	Hazard	Value

Methanol (*METHANOL SAFETY DATA SHEET*, n.d.)		Flammable		Health hazard	2
		Health hazard		Flammability	3
		Acute Toxic		Reactivity	0
Water (*Water Safety Data Sheet*, n.d.)	-	-		Health hazard	0
				Flammability	0
				Reactivity	0

6.1.4. Methanol Plant Safety

6.1.4.1. Explosion and Fire Control.

Methanol and its fumes are flammable, which poses a possible safety risk. The flash point is 12.2 degrees Celsius (closed cup), while the ignition temperature is 470 degrees Celsius. Methanol vapor is combustible at concentrations ranging from 5.5 to 44 vol%. At 20°C, the saturated vapor pressure is 128 kPa, making a saturated methanol-air combination combustible throughout a wide temperature range. The electrical conductivity of pure, anhydrous methanol is extremely low. When moving and handling methanol, precautions must be taken to avoid electrostatic charge (Ott et al., 2012).

6.1.4.2. Fire Prevention

Large storage facilities should have permanently installed fire-extinguishing equipment. Water cannons are commonly used in storage tank farms to keep steel structures and surrounding tanks cool in the case of a fire. Large tanks should have permanent piping systems for alcohol-resistant fire-extinguishing foams installed (Ott et al., 2012).

6.1.4.3. Fire Fighting

For small flames, conventional fire-extinguishing chemicals such as powder, carbon dioxide, or Halon can be employed.Because water is miscible with methanol, it cannot be used to extinguish flames involving substantial volumes of the methanol; combinations including tiny amounts of methanol may also ignite. Alcohol-resistant protein foams are appropriate. A methanol flame is nearly invisible in daylight, making firefighting more difficult. Although formaldehyde and carbon monoxide occur during burning when oxygen is limited, the methanol flame does not generate soot. When facing flames in confined locations, firefighters must use respirators (Ott et al., 2012).

6.1.4.4. Methanol Caused Incidents

An analysis of 81 distinct methanol accidents from 1998 to 2011 reveals that flames or explosions account for 81% of all incidents, while spills account for 14%. The transportation industry and industrial methanol users (including biodiesel producers) account for more than four out of every five recorded events, and 88% of all deaths (*METHANOL SAFE HANDLING MANUAL 4TH EDITION*, n.d.).

6.1.4.5. Methanol Tank Explosion and Fire at Bethune Point Wastewater Treatment Plant

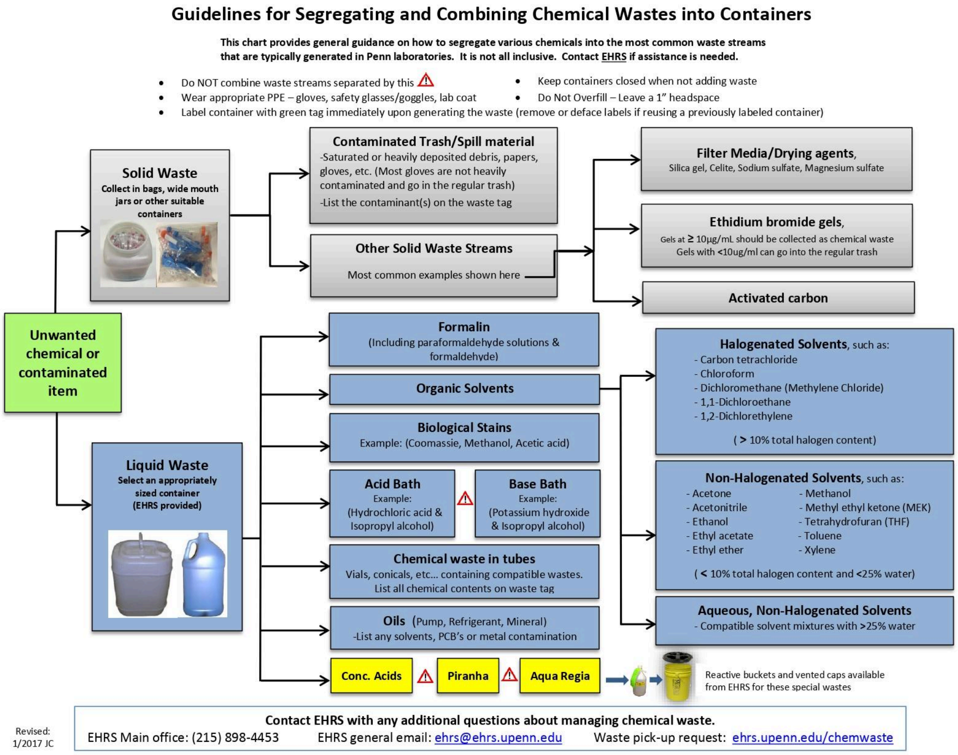
Three workers continued roof removal on Wednesday, January 11, 2006. The lead mechanic and the third worker were cutting the metal roof just over the methanol tank vent around 11:15 a.m. Sparks from the cutting torch ignited methanol fumes flowing from the vent, causing a fireball to form on top of the tank. The fire flashed past the vent's flame arrestor, igniting methanol fumes and air inside the tank, resulting in an explosion inside the steel tank (INVESTIGATION REPORT METHANOL TANK EXPLOSION AND FIRE, 2007).

6.2. Waste Streams

Table 6.2.1. Waste stream molar flow rates.

Mole Flows	**H2O1**	**H2O2**	**H2O3**	**Purge**
Total	4.90569	66.38379	9.098484	0.401186
CO2	0	0	0	0.342614
CO	0	0	0	0.002761

H2	0	0	0	0.007672
MEOH	4.453556	7.43772	6.444925	0
H2O	0.13536	58.47855	2.651301	0
N2	1.10E-02	0	0	0.002208
METHANE	9.64E-02	0	0	0.00482
DIMET-01	1.85E-01	1.10E-19	2.95E-29	0.009232
METHY-01	0.024189	3.90E-09	1.08E-12	0.008241
ACETO-01	0.000193	7.21E-11	1.75E-12	0.000133
ETHAN-01	0.000306	0.265985	0.002258	0.013428
1-PRO-01	1.69E-05	0.138946	0	0.006948
N-BUT-01	9.03E-07	0.062591	0	0.00313



Guidelines for Segregating and Combining Chemical Wastes into Containers

This chart provides general guidance on how to segregate various chemicals into the most common waste streams that are typically generated in Penn laboratories. It is not all inclusive. Contact EHRS if assistance is needed.

- Do NOT combine waste streams separated by this ⚠
- Wear appropriate PPE – gloves, safety glasses/goggles, lab coat
- Label container with green tag immediately upon generating the waste (remove or deface labels if reusing a previously labeled container)
- Keep containers closed when not adding waste
- Do Not Overfill – Leave a 1" headspace

Contact EHRS with any additional questions about managing chemical waste.

EHRS Main office: (215) 898-4453 EHRS general email: ehrs@ehrs.upenn.edu Waste pick-up request: ehrs.upenn.edu/chemwaste

Revised: 1/2017 JC

Figure 6.2.1. Guidelines for Segregating and Combining Chemical Wastes into Containers.

6.2.1. EPA Hazardous Waste

These specifically listed wastes are designated as F, K, P or U list. Acutely hazardous waste is designated by an H list hazard code and all P listed waste (*Hazardous Chemical Waste Defined*, n.d.).

The list includes waste that is either a processed waste or a discarded commercial product. A process waste is any waste that, by virtue of some use, process or procedure, no longer meets the manufacturer's original product specification. A discarded commercial chemical product is the original (virgin) material in the original container that is unwanted, unused or outdated (*Hazardous Chemical Waste Defined*, n.d.).

F003 Code-spent solvent mixtures and blends which contained, before use, a total of ten percent or more (by volume) of one or more of the following non-halogenated solvents: Xylene, Acetone, Ethyl acetate , Ethyl benzene, Methanol, Methyl isobutyl ketone, n-butyl alcohol, Cyclohexanone (*Hazardous Chemical Waste Defined*, n.d.).

Methanol (code is U154) is also classified as U-list chemical in epa hazardous waste codes, which means that it is discarded commercial chemical products, off-specification species, container residues, and spill residues thereof toxic wastes ("EPA HAZARDOUS WASTE CODES," n.d.).

6.2.2. Compatibility and Disposal Containers

Before different chemical wastes are mixed together in a single container for disposal, they should be for chemical compatibility and segregation. According to the RCRA's Chemical Waste Compatibility List ("RCRA's Chemical Waste Compatibility List," n.d.), no potential consequences are found from the components mixing in our waste streams (*Chemical Waste – USC Environmental Health & Safety*, n.d.).

The appropriate container should be selected for the waste stream according to (). Since the methanol water stream is aqueous solution, it should be kept in the Glass bottles, plastic bottles, plastic cans (*Chemical Waste – USC Environmental Health & Safety*, n.d.).

6.2.3. Waste management rules according to the Ministry of Ecology and Natural Resources of the Republic of Kazakhstan

Operations related to waste from the time of its creation to its final disposal are understood as waste management (*Қалдықтарды Басқару*, 2021).

For waste management operations:

1) accumulation of waste at the place of generation;

2) waste collection;

3) transportation of waste;

4) recovery of waste;

5) disposal of waste;

6) conducting monitoring of waste collection, transportation, recovery and (or) disposal operations;

7) includes services for disposal of destroyed (closed, decommissioned) waste disposal facilities.

6.2.4. Methanol in waste streams.

The waste stream from methanol production contains methanol along with water, impurities, and other organic compounds. This waste stream needs to be properly managed and treated to prevent environmental contamination and to potentially recover valuable resources. According to the US EPA Resource and Conservation Recovery Act (RCRA) reducing, reusing, and recycling methanol can significantly decrease the volume of methanol waste disposal, thus minimizing its environmental impact and reducing hazardous waste generation. (Methanol Fact Sheet)

Separation and purification. Initially, the waste stream would undergo separation processes to remove larger impurities and separate water from methanol and organic compounds. Distillation or other separation techniques can be employed for this purpose.

Storage. Similar to storing raw methanol, you can use tanks made of materials compatible with methanol to store the waste stream. These tanks should be properly labeled and stored in a well-ventilated area away from ignition sources.

Recovery. Purified methanol can then be reused in the production of the same site or for other production units nearby.

Treatment. Biological, chemical or physical treatments may be done to eliminate hazardous waste. For example, Conversion to higher-value chemicals such as methanol-to-olefins (MTO) or methanol-to-propylene (MTP). These conversion technologies allow for the production of ethylene, propylene, and other valuable chemicals from methanol, reducing waste and maximizing resource utilization.

Disposal. Once all of the options are fulfilled and there is still a small portion of any residual waste or treated effluent should be disposed of responsibly, in accordance with local regulations and environmental guidelines. This may involve further treatment to meet discharge standards or safe disposal methods such as incineration or landfilling.

VII. Total investment and Profitability

7.1. Market analysis of reactants and products

According to a recent market analysis, the global methanol market size was estimated at \$31.6 billion in 2022. It is expected to reach \$ 47.91 billion by 2032, with the growth rate of 5.1% (*Methanol Market*, n.d.).In terms of volume global methanol production is estimated at 90 million tonnes in 2022 and growth rate (CAGR) is expected to be at 4.3% (*Methanol Market*, n.d.). The rapidly expanding chemical industry, significant growth in the automotive industry, and the implementation of various government initiatives are some of the major factors propelling the market

The largest region in the methanol market is the Asia-Pacific, with an estimated \$ 21,239.4 million in 2022, the growth rate is at a CAGR of 5.2%. China is an undisputed major player in the market, as the data from 2021 shows \$3,860.11 million of imports. India is the second largest importer, with \$959.97 million.

7.2. Product specification and quality requirements

Methanol is a simple alcohol that is a colorless and tasteless liquid with a faint odor. There are different specifications and quality requirements for methanol depending on its application (for laboratory use or commercial use). In the United States, ASTM D1152 standard specification is used for methanol (*Standard Specification for Methanol (Methyl Alcohol)*, 2001). Methanol is classified as Grade A and Grade AA in ASTM specification. Grade AA is a more common standard for chemical use. IMPCA is another specification for methanol which was created in 1992 based on ASTM test methods (*ABOUT METHANOL*, n.d.). Nowadays, IMPCA specification is a common specification in most parts of the world.

Table 7.2.1. Commercial methanol product specifications according to ASTM D1152 and IMPCA standards.

Property	**ASTM D1152 Grade AA**	**IMPCA**
Methanol content, wt%	< 99.85	< 99.85
Water content, wt%	< 0.10	< 0.10
Ethanol content, mg/kg	< 10	< 50
Acetone content, mg/kg	< 20	< 30
Acetic acid content, mg/kg	< 30	< 30
Chloride as Cl^{-}, mg/kg	-	< 0.5
Sulfur, mg/kg	-	< 0.5
Total iron, mg/kg	-	< 0.1

As it can be seen from Table 7.2.1., these specifications have different requirements in terms of impurities like ethanol and acetone. However, both of these have the same purity requirement of < 99.85 wt%, which will be desired purity for our methanol production. Also, IMPCA will be our preferred specification because it is the most commonly used specification in the world.

7.3. Production rate selection

The main factor is this case, that should be acknowledged is that Kazakhstan’s demand for the methanol is not much dictated by the market demand, but rather the oil and gas companies using methanol as the raw material. Even though the data is limited, tendencies could be forecasted. The recent increase of production of high-octane benzene components led to the more demand for methanol import. The exemplary recent chemical plants are production of methyl tert-butyl ether (MTBE) by Shymkent Chemical Company and of tert-amyl methyl ether by Atyrau Oil refinery, has caused the increase in methanol demand by these companies

(Казахстан Увеличивает Закупки Метанола, 2023).Both plants have increased their methanol demand in 2022 compared to 2021, for 4.8 kT/yr and 3.4 kT/yr respectively (Казахстан Увеличивает Закупки Метанола, 2023).This tendency gives an important insight, that the methanol market in Kazakhstan is taking a similar step, as the major methanol countries, such as China, USA, or Russia, where the methanol is used mostly in production and forecasted to be in use more in the society in upcoming years. Also, this point serves as the justification for the calculation of the production capacity below.

It can be clearly seen that the methanol production grows each year, even despite the pandemics. Hence, it gives an opportunity to use the 2022 data as a benchmark for the calculation of the local methanol production, which is 111.02 million metric (*Statistic_id1323406_global-Methanol-Production-2017-2022*, n.d.). Then, to find the production rate in CIS, we use the following equation :

$$Production\ rate\ in\ CIS\text{:}\ \frac{GDP\ of\ CIS\ countries\ (excluding\ Russia)}{Global\ GDP} \times Production\ rate\ of\ the\ world$$

(7.3.1)

The overall GDP of CIS countries, excluding Russia, is 776.09 billion dollars (*Statistic_id268173_countries-with-the-Largest-Gross-Domestic-Product--Gdp--2022*, n.d.). The global GDP in 2022 was estimated to be 95 trillion dollars (*Statistic_id1347332_gdp-in-the-Cis-2022-by-Country*, n.d.). Hence, using the above mentioned equation:

$$Production\ rate\ in\ CIS\text{:}\ \frac{776.09\ billion\ dollars}{95\ trillion\ dollars} \times 111.02\ million\ metric\ tons\ =\ 0.907\ million\ metric\ tons$$

It was determined that the local methanol plant is expected to cover the 25% of the demand in CIS, hence, it also accounts for production, as by the demand-supply rule, we assume they are in equilibrium. Thus, we have a production rate for the local methanol:

$$25\%\ of\ the\ demand \times 0.907\ million\ metric\ tons\ =\ 0.22675\ million\ metric\ tons$$

, which accounts for 223.17 kilotons. Production rate is also adjusted by the average catalytic activity of 89%, as the catalyst is the important part of the whole process (Ogle A. & Carpeter R. Andrew, 2014):

$$226.75\ kilotons\ *\ 89\%\ =\ 201.8075\ kT/year$$

For forecasting, we keep the assumption, that due to the similar GDP growth rates of global and CIS countries will remain the same throughout the years, we can keep the ratio same for the upcoming years, hence, the production rate will be calculated the same for the upcoming years for the local plant:

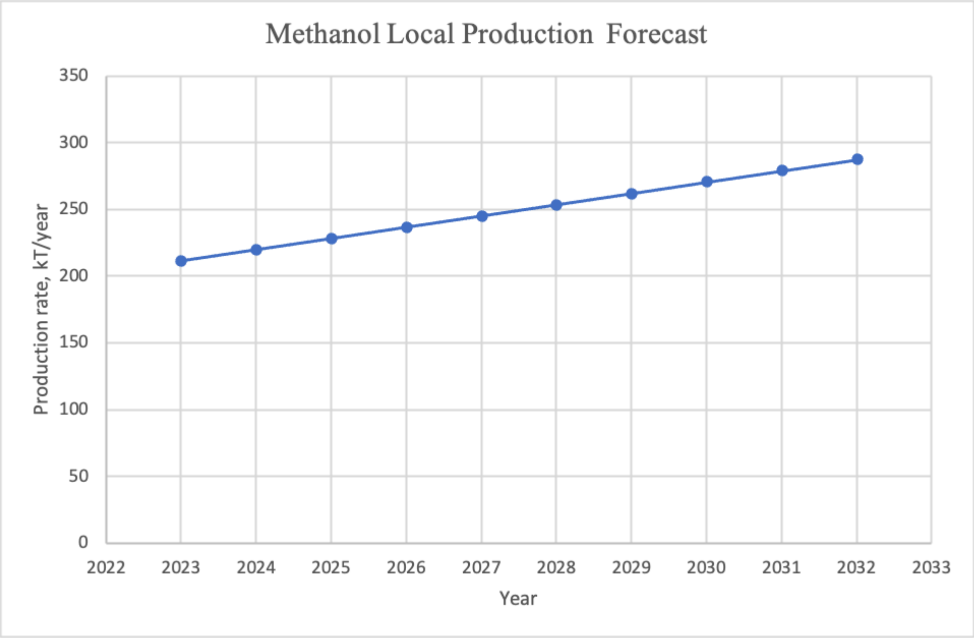


Figure 7.3.1 Methanol Local Production Forecast

For the year 2025, the forecasted value is 227.86 kT/year, while for the year 2030 it is 270.015 kT/year, so the chemical plant is expected to produce more methanol each year.

7.4. Cost estimation

Capital cost refers to the total amount of money that an investor or business needs to invest initially to initiate a project or venture. To find it the fixed and variable costs were estimated from the Aspen Process Economic Analyzer (APEA) and summed up. The calculations with formulas were performed in Excel.

7.4.1. Components of Capital Cost

Inside Battery Limits (ISBL) plant investment

ISBL is the cost of everything that is inside the plant, in our case the equipment and installation costs were considered to find it. ISBL cost is 35,267,000 USD, total equipment cost with total installation cost.

Offsite (OSBL) Investment

Offsite (OSBL) Investment includes additions to site infrastructure, boilers, electric sub-stations, shipping facilities, docks, laboratories, offices . It is often approximated as 40% of ISBL cost as first approximation, which will be 14,106,800 USD.

ISBL + OSBL = fixed capital = 49,373,800 USD.

Engineering Costs are given in Table 7.4.1.

Table 7.4.1. Engineering Summary from APEA.

ENGINEERING SUMMARY	**Cost, USD**	**Manhours**
Basic Engineering	750,400	6198
Detail Engineering	1,450,000	12970
Material Procurement	576,200	
Home Office	144,200	1381
Total Design, Eng, Procurement Cost	2,920,000	

7.4.2. Order of magnitude estimates

Equations 7.2 and 7.3 from the Towler and Sinnott (2021) textbook were used to estimate the capital costs.

$$C_2 = \frac{C_1}{S_1^n} \times S_2^n = aS_2^n \tag{7.4.1}$$

$$\frac{C_2}{S_2} = aS_2^{n-1} \tag{7.4.2}$$

where C_2 = ISBL capital cost the plant with capacity S2
C_1 = ISBL capital cost of the plant with capacity S1

For the Methanol via steam reforming & synthesis by Davy Process Tech. licensor, the exponent n is 0.6, the parameter a is 2775, Supper is 7000, Slower is 3000. Calculated C_2 was 562, 758.

7.4.3. Estimating Equipment Costs

Equipment Costs were given in Aspen Process Economic Analyzer (APEA) and are listed in Table 7.4.2.

Table 7.4.2. Equipment Costs.

Component Name	**Component Type**	**Total Direct Cost**	**Equipment Cost**
		(USD)	(USD)

H-101	DHE TEMA EXCH	353,800	92,900
D-103-cond	DHE TEMA EXCH	613,300	370,000
D-103-cond acc	DHT HORIZ DRUM	268,000	47,700
D-103-reb	DRB U TUBE	550,500	263,300
D-103-reflux pump	DCP CENTRIF	100,600	21,600
D-103-tower	DTW TOWER	2,320,000	1,490,000
HE-101	DHE TEMA EXCH	403,000	42,200
CL-101	DHE TEMA EXCH	554,900	277,200
S-101	DVT CYLINDER	171,600	59,000
R-101	DAT REACTOR	749,900	481,700
D-102-cond	DHE TEMA EXCH	614,800	371,500
D-102-cond acc	DHT HORIZ DRUM	268,000	47,700
D-102-reflux pump	DCP CENTRIF	100,600	21,600
D-102-tower	DTW TOWER	2,860,000	1,860,000
C-101	DGC CENTRIF	2,530,000	2,270,000
D-101-cond	DHE TEMA EXCH	83,200	13,900
D-101-cond acc	DHT HORIZ DRUM	125,100	18,200
D-101-reb	DRB U TUBE	112,900	22,100
D-101-reflux pump	DCP CENTRIF	37,500	6000
D-101-tower	DTW TOWER	307,700	99,700
	Total equipment cost		**7,880,000**

7.4.4. Estimating Installed Costs

Chemical process plant capital cost estimates are frequently predicated on an estimation of the cost of purchasing the principal equipment components needed for the process; other costs are estimated as components of the equipment cost (Towler & Sinnott, 2021).

Lang (1948) suggested that the ISBL fixed capital cost of a plant is given as a function of the total purchased equipment cost by the equation (Towler & Sinnott, 2021):

$$C = F(\Sigma C_e) \tag{7.4.1}$$

where C = total plant ISBL capital cost (including engineering costs)

ΣCe = total delivered cost of all the major equipment items: reactors, tanks, columns, heat exchangers, furnaces, etc.

F = an installation factor,later widely known as a Lang factor

Lang originally proposed the following values of F, based on 1940s economics:
F = 3.1 for solids processing plant
F = 4.74 for fluids processing plant
F = 3.63 for mixed fluids-solids processing plant

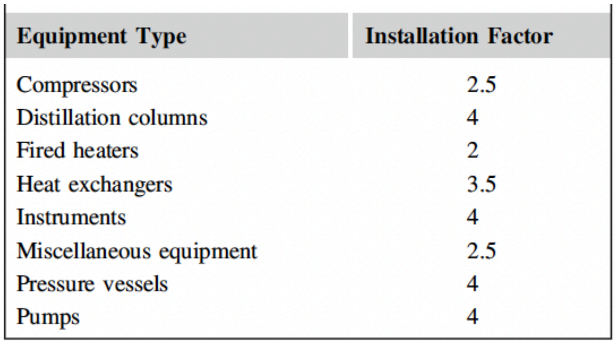
C is 14,800,000 USD, the calculated ΣCe was 7,880,000 USD, so the F is 1.88.

Factorial Estimates

By taking into account each of the cost components that are compounded into the Lang factor separately, the installation factor can also be approximated with a little more precision (Towler & Sinnott, 2021). Using the equation 7.4 below, the installation costs for each equipment can be calculated based on Table 7.4.3 from the Towler and Sinnott (2021) textbook.

$$C_{installed} = C_{equip} * F \qquad (7.4.2)$$

Table 7.4.3. Installation Factors Proposed by Hand (1958) (Towler & Sinnott, 2021).



Equipment Type	Installation Factor
Compressors	2.5
Distillation columns	4
Fired heaters	2
Heat exchangers	3.5
Instruments	4
Miscellaneous equipment	2.5
Pressure vessels	4
Pumps	4

The results are given in Table 7.4.4.

Table 7.4.4. Installation costs of the equipment.

Component Name	C, Installed costs	F, Installation factors
H-101	185,800	2
D-103-cond	1,480,000	4
D-103-cond acc	190,800	4
D-103-reb	1,053,200	4

D-103-reflux pump	86,400	4
D-103-tower	5,980,000	4
HE-101	148,000	3.5
CL-101	693,000	2.5
S-101	147,500	2.5
R-101	1,926,800	4
D-102-cond	1,486,000	4
D-102-cond acc	190,800	4
D-102-reflux pump	86,400	4
D-102-tower	7,430,000	4
C-101	5,670,000	2.5
D-101-cond	55,600	4
D-101-cond acc	72,800	4
D-101-reb	88,400	4
D-101-reflux pump	24,000	4
D-101-tower	398,800	4
Total installation cost	**2.74E+07**	

7.4.4. Materials Selection characteristics

Many aspects must be taken into account while choosing engineering materials for the equipment. For the chemical process plant high temperature strength and corrosion resistance are typically the most important factors to take into account. The process engineer must also take the mechanical specifications into account; the material used must be easily worked and have adequate strength. The least expensive material that satisfies mechanical and process requirements should be chosen; this is the material that will result in the lowest cost over the plant's operational life, permitting replacement and maintenance. Next the material selection characteristics and process will be described according to the (Towler & Sinnott, 2021).

The main essential characteristics for material choice:

1. Mechanical properties;
2. The effect of high temperature, low temperature, and thermal cycling on the mechanical properties;
3. Corrosion resistance;
4. Any special properties required, such as thermal conductivity, electrical resistance, magnetic properties;
5. Ease of fabrication—forming, welding, casting;
6. Availability in standard sizes—plates, sections, tubes;
7. Cost.

7.4.5. Materials Selection

The most widely utilized corrosion-resistant materials in the chemical sector are stainless steels. It was chosen as a material for equipment for the methanol production plant. Mechanical characteristics of the stainless steel are described below.

There is a large selection of stainless steels available, each with a composition designed to provide the qualities needed for a particular use. Based on their microstructure, they can be categorized into three major classes:

1. Ferritic: no nickel, <0.1% C, 13–20% Cr
2. Austenitic: >7% Ni, 18–20% Cr
3. Martensitic: 0.2 to 0.4% C, up to 2% Ni, and 12–14% Cr

In order to achieve corrosion resistance, Austenite's uniform structure (a face-centered cubic structure with carbides in solution) is what is desired. Table 7.4.5.displays the composition of the major grades of austenitic steels. Their properties are discussed below.

Type 304 (18/8 stainless steels): the stainless steel that is most generally used. It has the lowest amounts of Ni and Cr necessary to provide a stable austenitic structure.

Because of the low carbon concentration, thin sections typically don't require heat treatment to avoid weld decay.

Type 304L: A low-carbon (<0.03% C) variant of type 304, intended for thicker welded sections where type 304 would cause carbide precipitation.

Type 321: A titanium-stabilized variant of 304 designed to stop carbide precipitation during welding. It is better suited for usage in high temperatures and has a little higher strength than 304L.

Type 347: Stabilized with niobium.

Type 316: Molybdenum is added to this alloy to increase its resistance to corrosion in reducing conditions, such as diluted sulfuric acid and, more specifically, solutions containing chlorides.

Type 316L: is a low-carbon variant of type 316 that needs to be mentioned if heat treatment or welding could result in the precipitation of carbide in type 316.

Types 309/310: Chromium-rich alloys, which offer improved oxidation resistance at high temperatures. At temperatures higher than 500C, sigma phase production can cause embrittlement in alloys containing more than 25% Cr. FeCr is an intermetallic compound found in sigma phase.

Table 7.4.5. Commonly used grades of austenitic stainless steel.

Specification No	Compositions %							
	C max	Si max	Mn max	Cr range	Ni range	Mo Range	Ti	Nb
304	0.08		2	17.5-20	8-11			
304L	0.03	1	2	17.5-20	8-12			
321	0.12	1	2	17-20	9-12		4*C	
347	0.08	1	2	17-20	9-13			10*C
316	0.08	1	2	16-18	10-14	2-3		
316L	0.03	1	2	16-18	10-14	2-3		
309	0.20			22-24	12-15			
310	0.25			24-26	19-22			

A material's fundamental strength is determined by its tensile strength, often known as its tensile stress. It is the highest stress that the material can bear, as determined by a typical tensile test. Proof stress, typically 0.1%, is the amount of stress necessary to generate a given permanent deformation. If the material is under stress, the rate of corrosion can be altered.

In normal design stress values, the rate of impact will typically not alter considerably. However, a phenomena known as stress corrosion cracking can happen for specific metal, corrosive agents, and temperature combinations. This is the broad term for an attack when fast-growing cracks are created, which may lead to the metal breaking too soon and brittlely.

Table 7.4.6. Mechanical properties of the stainless steel.

	Tensile Strength (N/mm^2)	0.1% proof Stress (N/mm^2)	Modulus of Elasticity (kN/mm^2)
Stainless steel	>540	200	210

The carbon steel is also one of the good options for the equipment material, however, all types of the austenitic stainless steels have greater strength than the plain carbon steels. I can be concluded from table 7.4.7. , which demonstrates the tensile strength values of the carbon and stainless steels.

Table 7.4.7. Minimum tensile strength, maximum temperature and maximum allowance stress of materials.

Material	Grade	Min tensile Strength (N/mm^2)	Maximum temperature (C)	Maximum allowable Stress (ksi [1ksi=6.8948 N/mm^2]) at Temperature (C)				
				38 (100 F)	149 (300F)	260 (500F)	371 (700F)	482 (900F)
Carbon steel	A285	310.264	482	12.9	12.9	12.9	11.5	5.9
Stainless steel 13% Cr	410	448.159	649	18.6	17.8	17.2	16.2	12.3
Stainless steel 18% Cr, 8% Ni	304	517.107	815	20.0	15.0	12.9	11.7	10.8
Stainless steel 18% Cr, 10% Ni, Cb	347	517.107	815	20.0	17.1	15.0	13.8	13.4
Stainless steel 18% Cr, 10% Ni, Ti	321	517.107	815	20.0	16.5	14.3	13.0	12.3
Stainless steel 16% Cr,	316	517.107	815	20.0	15.6	13.3	12.1	11.5

12% Ni, 2% Mo								

The design temperature is always the basis for determining the maximum permissible stress in a given design. The right materials must be selected in order to provide a wall thickness that is both mechanically and economically feasible at the design temperature. In this regard, stainless steels are better than regular carbon steels.

The higher the alloying prercentage, the better the corrosion resistance over a wide range of conditions, strongly oxidizing to reducing, but the cost will be higher.

Chromium is the most effective alloying element to give resistance to oxidation, forming a tenacious oxide film. Chromium alloys should be specified for equipment subject to temperatures above 480C in oxidizing atmospheres. For example, type 410 stainless steel (13% Cr) can be used up to 650C (1200F). (Table 7.4.7)

The chromium percentage of an alloy must be greater than 12% in order to confer corrosion resistance; the higher the chromium concentration, the more resistant the alloy is to corrosion under oxidizing circumstances. To increase corrosion resistance in nonoxidizing conditions, nickel is used.

The following is a ranking of corrosion resistance, with type 304 being at the top:

Table 7.4.8. Corrosion resistance of austenitic stainless steel.

Stainless steel types	304	304L	321	316	316L	310
Corrosion resistance	1.0	1.1	1.1	1.25	1.3	1.6

When choosing stainless steel types appropriate for usage in a given environment, one must take into account the problem of intergranular corrosion, also known as weld decay.

According to Table 7.4.8 the corrosion resistance of all the austenitic stainless steel is higher than the 304 type.

Table 7.4.9 provides an indication of the price of some regularly used metals. The real price of metals and alloys will vary greatly based on changes in global metal markets. When evaluating material costs, one must consider the material density and strength (maximum permitted stress), as these will determine the quantity of a material used. According to Table X5 the carbon steel is the cheapest option of material, however, it is less effective than materials with a relatively high maximum permissible stress, such as stainless and low alloy steels.

Table 7.4.9. Relative cost of metals.

Metal	Type or grade	Price ($/lb) (1 lb=0.45 kg)	Max allowable stress (ksi) at 40C (100F)	Relative cost rating
Carbon steel	A-285	0.27	12.9	1
Austenitic stainless steel	304	1.90	20	2.2
	316	1.64	20	4
Aluminum alloy	A03560	1.27	8.6	2.4
Copper	C10400	3.34	6.7	27
Nickel	99%Ni	8.75	10	48
Incoloy	N08800	3.05	20	7.5
Monel	N04400	6.76	18.7	20
Titanium	R50250	9.62	10	27

Considering and comparing the main characteristics such as mechanical properties, corrosion resistance and the cost, it is concluded that stainless steel is the best material for the plant equipment.

7.4.6. Materials Cost Factors

The installation factors given in Tables 7.4 and 7 5 in the Towler and Sinnott (2021)textbook are for plants built from carbon steel. Materials factor fm should be introduced in our case since the materials used in our plant also include 304 stainless steel, the material cost factor of which is 1.3, according to the table 7.4.11.

Table 7.4.10. Typical Factors for Estimation of Project Fixed Capital Cost (Towler & Sinnott, 2021).

Item	Process Type		
	Fluids	Fluids–Solids	Solids
Major equipment, total purchase cost	C_e	C_e	C_e
f_{er} Equipment erection	0.3	0.5	0.6
f_p Piping	0.8	0.6	0.2
f_i Instrumentation and control	0.3	0.3	0.2
f_{el} Electrical	0.2	0.2	0.15
f_c Civil	0.3	0.3	0.2
f_s Structures and buildings	0.2	0.2	0.1
f_l Lagging and paint	0.1	0.1	0.05
ISBL cost, $C = \Sigma C_e \times$	3.3	3.2	2.5
Offsites (OS)	0.3	0.4	0.4
Design and Engineering (D&E)	0.3	0.25	0.2
Contingency (X)	0.1	0.1	0.1
Total fixed capital cost $C_{FC} = C\,(1 + \text{OS})(1 + \text{D\&E} + \text{X})$			
$= C\times$	1.82	1.89	1.82
$= \Sigma C_e\times$	6.00	6.05	4.55

Table 7.4.11. Materials Cost Factors, f_m, Relative to Plain Carbon Steel (Towler & Sinnott, 2021).

Material	f_m
Carbon steel	1.0
Aluminum and bronze	1.07
Cast steel	1.1
304 stainless steel	1.3
316 stainless steel	1.3
321 stainless steel	1.5
Hastelloy C	1.55
Monel	1.65
Nickel and Inconel	1.7

$$f_m = \frac{\text{purchased cost of item in exotic material}}{\text{purchased cost of item in carbon steel}} \qquad (7.4.3)$$

f_m is not equal to the ratio of the metal prices, as the equipment purchased cost also includes labor costs, overheads, fabricator’s profit, and other costs that do not scale directly with metal price. Equation 7.4.3 can then be expanded for each piece of equipment give:

$$C = \sum_{i=1}^{i=M} C_{e,i,CS}[(1 + f_p)f_m + (f_{er} + f_{el} + f_i + f_c + f_s + f_l)] \qquad (7.4.5)$$

where
Ce,i,CS = purchased equipment cost equipment i in carbon steel
Ce,i,A = purchased equipment cost equipment i in alloy
M= total number of pieces of equipment
fp = installation factor for piping
fer = installation factor for equipment erection
fel = installation factor for electrical work
fi = installation factor for instrumentation and process control
fc = installation factor for civil engineering work
fs = installation factor for structures and buildings
fl = installation factor for lagging,insulation,or paint.

Equation 7.4.5 should be used when the purchased equipment cost has been found on a carbon steel basis and the designer is estimating the cost for alloy construction. If the purchased equipment cost has been obtained on an alloy basis, then the designer should instead correct the other installation factors so as not to overestimate the cost of installation:

The following materials were used for our equipments:

Table 7.4.12. Materials of the equipment.

Unit	Material	fm
All units	304 stainless steel	1.3

As a result, the calculated total installation cost considering the material factors is **29,456,614 USD**.

7.4.6. Updating cost estimates

Every cost-estimating technique anticipates future expenses based on historical data. Inflation affects both the cost of labor and the prices of building materials. In order to estimate during the design phase and project the plant's future construction costs, some technique must be employed to update historical cost data.

Published cost indices are a component of the standard procedure used to update historical cost data. These are based on labor, material, and energy cost statistics that are released in government statistical digests and connect current costs to historical expenses. The formula 7.8 and Figure 7.4.1 from the Towler and Sinnott (2021) textbook is used to calculate the cost of our plant if it was installed in 2008. Since the cost index in year 2008 is approximately 600 and in year 2000 is around 400, the cost in year 2000 was calculated using the time value of money formula:

$PV = \frac{FV}{(1+r)}$, where PV - present time value, FV - future value, r - rate of interest. The interest rate in Kazakhstan is 14.75% (TRADING ECONOMICS, n.d.).

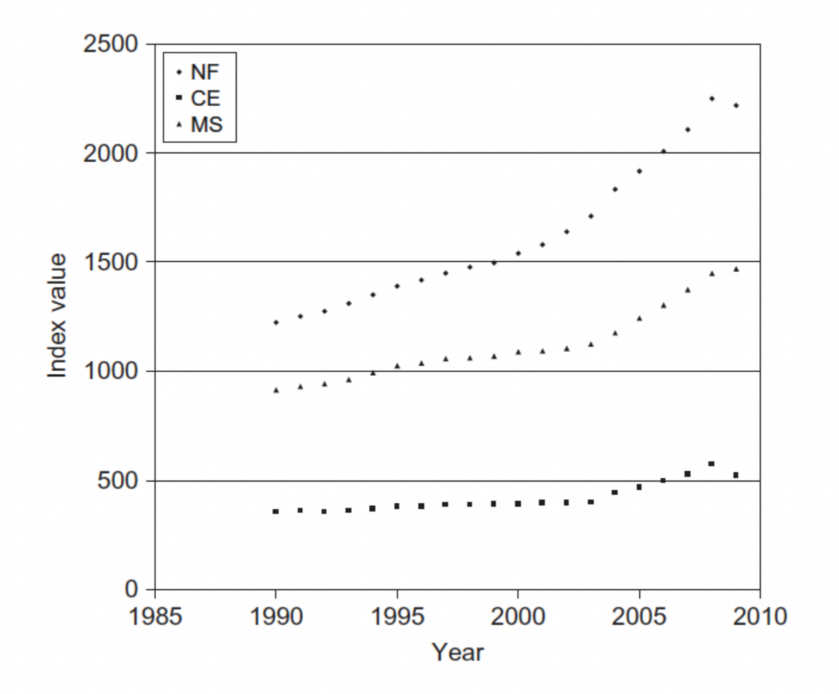


Figure 7.4.1. Variation of major cost indices (Towler and Sinnott (2021).

$$Cost\$_{20XX} LocationB = Cost\$_{2000} LocationA * \frac{Cost\ Index\ 20XX}{Cost\ Index\ 2000} * \frac{Location\ Index\ B}{Location\ Index\ A} \quad (7.4.6)$$

The results are given in Table 7.4.13.

Table 7.4.13. The calculated values of updated cost estimates.

Cost in year 2008	19,300,000 $
Cost in year 2000	12,900,000 $
Cost index in year 2008	600 $
Cost index in year 2000	400 $
Cost in year 2024	14,800,000 $
Cost in year 2000	12,900,000 $

7.5. Plant Economics

Plant Economics of the Methanol Production plant was performed in Excel, based on the Peters (2004) textbook.

Table 7.5.1. Syngas data.

Raw Materials	Products	Byproducts	Waste
Syngas	Methanol	None	Hydrogen, Nitrogen, Carbon monoxide, Carbon dioxide, Water, Methane, Dimethyl ether (DME), Methyl formate, Acetone, Ethanol, Propanol, Butanol

7.5.1. Project Cash Flows

The projected cash flows from the APEA document were plotted and demonstrated in Figure 7.4.2. It shows negative values since Aspen gives us estimated Cash Flows.

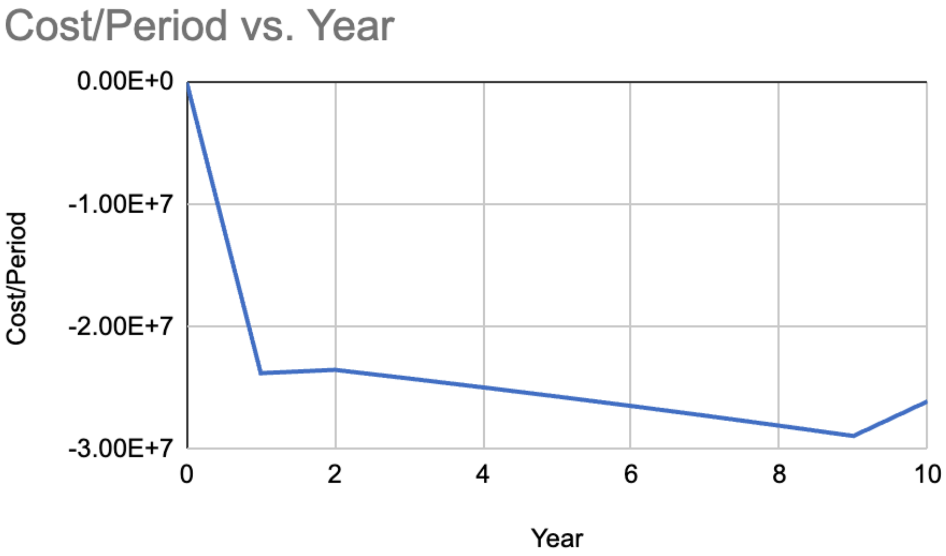


Figure 7.4.2. Cost/Period vs. Year plot

7.5.2. Simple Measures of Economic Return

Throughout the course of a project, cash flows are initially expended by the company to cover expenses such as engineering, equipment acquisition, plant construction, and the initiation of plant operations. Following the completion of construction and the commencement of operations, revenue generated from product sales starts to enter the company's coffers.

7.5.2.1. Pay-back time

The payback period is a crucial metric in evaluating investments, representing the time it takes for an investment to recoup its initial cost through cash flows. The payback period signifies the point in time when these incoming cash flows match or surpass the initial investment, marking the project's break-even point. It serves as a valuable tool for assessing the feasibility and risk of an investment, providing insights into the speed of return and liquidity of the venture. To calculate pay-back time the Equation 7.1 below was used.

$$Simple\ pay - back\ time = \frac{Total\ investment}{Average\ annual\ cash\ flow} \tag{7.5.1}$$

The payback period of our plant is 5 years.

7.5.2.2. Return on investment

Return on Investment (ROI) is a financial metric used to evaluate the profitability of an investment. It's calculated by dividing the net profit generated by the investment by the initial cost of the investment, and then expressing the result as a percentage.

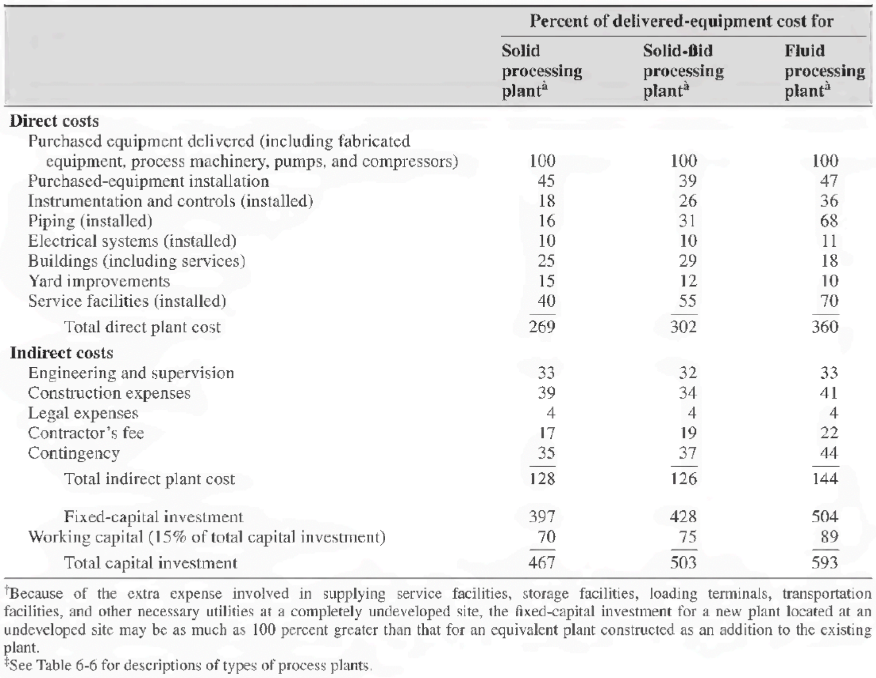
$$Return\ on\ investment = \frac{Net\ annual\ profit}{Total\ investment} \tag{7.5.2}$$

The ROI of our plant is 3,350,000 %/y.

7.5.2.4. Estimation of capital investment by percentage of delivered equipment method

Capital Investment was estimated using Table 6-9 in Peters (2004) book, the fractions of delivered equipment were already given, fluid processing plant values were chosen. The direct costs,indirect costs, fixed capital investment (FCI) were calculated by multiplying those fractions to purchased equipment cost taken from Aspen Economics (APEA). The calculations are in Excel, as a result, the estimated values of capital investment in million USD units were shown.

Table 7.5.2. Ratio factors for estimating capital investment items based on delivered- equipment cost.



	Percent of delivered-equipment cost for		
	Solid processing plant[a]	**Solid-fluid processing plant**[a]	**Fluid processing plant**[a]
Direct costs			
Purchased equipment delivered (including fabricated equipment, process machinery, pumps, and compressors)	100	100	100
Purchased-equipment installation	45	39	47
Instrumentation and controls (installed)	18	26	36
Piping (installed)	16	31	68
Electrical systems (installed)	10	10	11
Buildings (including services)	25	29	18
Yard improvements	15	12	10
Service facilities (installed)	40	55	70
Total direct plant cost	269	302	360
Indirect costs			
Engineering and supervision	33	32	33
Construction expenses	39	34	41
Legal expenses	4	4	4
Contractor's fee	17	19	22
Contingency	35	37	44
Total indirect plant cost	128	126	144
Fixed-capital investment	397	428	504
Working capital (15% of total capital investment)	70	75	89
Total capital investment	467	503	593

[†] Because of the extra expense involved in supplying service facilities, storage facilities, loading terminals, transportation facilities, and other necessary utilities at a completely undeveloped site, the fixed-capital investment for a new plant located at an undeveloped site may be as much as 100 percent greater than that for an equivalent plant constructed as an addition to the existing plant.

[‡] See Table 6-6 for descriptions of types of process plants.

7.5.2.5. Annual operating labor and material costs

The plant produces methanol as a product and consumes syngas as a raw material. The price for syngas is 0.102 USD/Nm^3 (Alerts, n.d.) which is 0.09 USD/kg, since Gas laws state that 1 Nm3 of syngas at standard conditions is approximately 1.18 kg. The methanol price is 380 USD/MT, which is 0.38 USD/kg (*How Much Is 1.77 Nm3 Syngas in Kg? | 5 Answers From Research Papers*, n.d.). They were used to calculate annual value of product and raw materials.

Annual operating labor costs include operating labor and supervision, according to Aspen APEA. The number of operations per shift for operators is 4, for supervisors is 1. The average operator rate was chosen as 250000 in average tg/month, which is 561.53 USD/month (*Вакансия Оператор Производственной Линии В Астане, Работа В Компании EcoTara*, 2024). Summing them up, the annual operating labor costs were calculated. The results are given in Table 7.5.3.

Table 7.5.3. The annual operating labor and material costs.

Total annual value of products, million $/y	76.69
Total annual cost of raw materials, million $/y	23.16
Annual operating labor cost, million $/y	0.595

These values were further needed to estimate the Annual Total Product Cost (TPC).

7.5.2.6. Annual Total Product Cost

Total Product Cost Without Depreciation = Variable Cost + Fixed Charges + Plant Overhead + Manufacturing Cost+General Expense = 7,329,622 million USD/year.

Variable Cost includes Raw Materials, Operating Labor, Operating Supervision, Utilities, Maintenance and Repairs, Operating supplies, Laboratory charges, Royalties.]

Fixed Charges includes Taxes, Financing, Insurance, Rent, Depreciation.

General Expense is the sum of Administration, Distribution & Selling, Research & development Costs.

Utilities

In Aspen APEA, the utilities that were used for the plant are electricity, cooling wastewater, and steam. The electricity rate costs were taken for Kazakhstan, which is 0.11 USD per kWh. The annual utility costs are given in Table 7.5.4.

Table 7.5.4. The annual utility costs.

Electricity, million $/y	0.000354
Cooling wastewater, million $/y	5.743
Steam, million $/y	4.491

7.5.3.Taxes and Depreciation

Corporations are obligated to pay taxes on their income, a requirement that varies depending on the country and is subject to yearly updates within the tax code. For instance, in Kazakhstan, the current tax system imposes a rate of 20%. Additionally, beyond income taxes, corporations may also be liable for municipal taxes and other related fees.

The U.S. Tax Reform Act of 1986 established the MACRS depreciation system. IRS document 946 contains information on the MACRS depreciation technique. In essence, the approach combines the straight-line and declining-balance methods. The MACRS approach shifts to charging the same amount as the straight-line method when the depreciation charge is less than it would be under the straight-line method. Until then, the declining-balance method is employed (Towler & Sinnott, 2021).

Different recovery durations are allocated to various asset classes under MACRS depreciation, depending on a usable life (also known as "class life") that is determined by the US Internal Revenue Service (IRS). At the time of writing, the IRS publication 946, the most recent version, specifies a 5-year recovery period and a 9.5-year class life for chemicals manufactured (Towler & Sinnott, 2021).

One further significant convention related to MACRS depreciation is that the technique gives half of the complete year's depreciation to the first and final years of the recovery period, based on the assumption that all property is acquired in the middle of the year (Towler & Sinnott, 2021).

The Total Depreciation Expense according to APEA is 14,799,800 USD per year. The Depreciacion in the Excel was calculated using MACRS depreciation method.

7.5.4. Time Value of Money

Time value of money refers to the principle that money available today is worth more than the same amount in the future, due to its potential earning capacity. To calculate it the future worth was estimated and Equation 7.8 was used.

$$present\ value\ of\ future\ sum\ =\ \frac{future\ worth\ in\ year\ n}{(1+i)^n} \qquad (7.5.3)$$

7.5.5. Discounted Cash Flow Methods

To find the present value of future cash flow the Equation 7.9 was used.

$$NPV = \sum_{n=1}^{n=t} \frac{CF_n}{(1+i)^n} \qquad (7.5.4)$$

Where,

CF_n - cash flow in year n,

t -project life.

The "discounted cash-flow rate of return" (DCFROR) also known as IRR was calculated using Equation 7.10 to find the maximum interest rate that a project could yield and still achieve break-even status by the conclusion of its life cycle.

$$\sum_{n=1}^{n=t} = \frac{CF_n}{(1+i')^n} = 0 \qquad (7.5.5)$$

Where,

CFn - cash flow in year n,
t - project life in years,
i′ - the discounted cash-flow rate of return (percent/100).

Table 7.5.5. Discounted Cash Flow Data.

Profitability measures, time value of money NOT included:		**Profitability measures including time value of money, with ANNUAL END-OF-YEAR cash flows and discounting**		**Profitability measures including time value of money, with CONTINUOUS cash flows and discounting**	
Return on investment, ave. %/y	3,350,000	Net present worth, 106$ =	772,000,000	Net present worth, 106$ =	829,000,000
Payback period, y	5.12	Discounted cash flow rate of return, DCFR, %/y =	15.2	Discounted cash flow rate of return, DCFR, %/y =	14.1
Net return, 106$	-3.19E+13				

7.5.6. Annualized Costs

Annualized costs were calculated to compare a current capital expense with a future cash flow by converting the initial capital expenditure into a recurring annual charge. This approach allows for a more straightforward comparison by breaking down the upfront cost into manageable yearly payments.

$$ACCR = \frac{A}{P} = \frac{[i(1+i)^n]}{(1+i)^n-1} = \frac{[0.1525(1+0.1525)^3]}{(1+0.1525)^3-1} = 0.4398 \qquad (7.5.6)$$

Annual cost = ACCR × Initial cost = 0.4398 ×481,700 = \$211,848

VIII. Conclusion and future work

8.1. Conclusion and future work

To sum up, the capstone project has successfully accomplished its main goal - designing the methanol plant which would operate in Kazakhstan, using syngas as the raw material. Throughout the project, the major and minor equipment, catalyst and its composition, production rate, and other important factors were evaluated and selected. Analyzing the transportation networks, market access and raw material availability, the location was chosen to be the Atyrau region. This location is also advantageous as it is included into the tax-free Special Economic Zone, which offers great opportunities for constructing and investing into the plant. The resultant process flow diagram consists of five major equipment: reactor, heat exchanger and three distillation columns. With the successful design of the whole process, the final product totally satisfies the purity and water content requirements. With the optimization of the distillation column arrangement, it was possible to decrease the methanol mass flow rate in the waste streams, which made it possible to produce high-purity methanol efficiently. Accordingly, all of the objectives set in the initial stages of work were completed successfully.

- Literature review on manufacturing options;
- Selection and justification of a production rate;
- Analysis of the properties of pure components and mixtures;
- Analysis of the security measures of the selected process and involved chemicals;
- Designing the process flow diagram and major/minor equipments

The future work could include several improvements to the overall process. First of all, some economic optimization is applicable, as it could be possible to reduce the operating costs, find cheaper raw material, or receive subsidies from the government. Secondly, the process itself could be adjusted too, for example the design of the distillation columns could be improved more, to increase the purity and decrease the methanol mass flow rate in the waste streams. Thirdly, market access could be reevaluated due to the economic and social changes. It could be achieved through more thorough market analysis and identification of the potential customers in CIS. The current location offers a possibility to export the methanol through the automobile roads, railroads and sea transportation, so all of these could be incorporated into the sales management after launching the plant. Overall, the current project is well-designed and ready to operate in the near future.