TECHNO-ECONOMIC ANALYSIS OF ACETONE AND ETHYLENE PRODUCTION FROM
BIOETHANOL

Miss Thanyarath Nueangchamnong

จุฬาลงกรณ์มหาวิทยาลัย
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การวิเคราะห์เทคโนโลยีและเศรษฐศาสตร์ของการผลิตแอซิโทนและเอทิลีนจากไบโอเอทานอล

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By	Miss Thanyarath Nueangchamnong
Field of Study	Chemical Engineering
Thesis Advisor	Assistant Professor PONGTORN CHAROENSUPPANIMIT, Ph.D.

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--------------------------------- Dean of the FACULTY OF ENGINEERING

(Professor SUPOT TEACHAVORASINSKUN, D.Eng.)

THESIS COMMITTEE

--------------------------------- Chairman

(Professor TAWATCHAI CHARINPANITKUL, D.Eng.)

--------------------------------- Thesis Advisor

(Assistant Professor PONGTORN CHAROENSUPPANIMIT, Ph.D.)

--------------------------------- Examiner

(Associate Professor APINAN SOOTTITANTAWAT, D.Eng.)

--------------------------------- External Examiner

(Associate Professor Atichat Wongkoblap, Ph.D.)

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การใช้งานหลักของไบโอเอทานอล คือการเป็นส่วนผสมในน้ำมันเบนซินหรือเรียกว่า "น้ำมันแก๊สโซฮอล์" ซึ่งช่วยลดการพึ่งพาเชื้อเพลิงธรรมชาติ อีกทั้งเป็นการลดการนำเข้าน้ำมันดิบจากต่างประเทศ และเป็นการสนับสนุนภาคการเกษตร เนื่องจากวัตถุดิบหลักในการผลิตไบโอเอทานอล คือมันสำปะหลัง และอ้อย ปัจจุบันประเทศไทยมีแนวโน้มการเติบโตของปริมาณรถยนต์ไฟฟ้า (EVs) อย่างต่อเนื่องจากมาตรการของรัฐบาล สำหรับรถยนต์ไฟฟ้าที่มีการผลิตภายในประเทศ และบริษัทที่มีแผนในการจัดตั้งฐานการผลิตในประเทศ ทำให้ไบโอเอทานอลในประเทศกำลังเผชิญความท้าทายหลายประการ เช่น ความต้องการที่ลดลงจากแนวโน้มการเพิ่มขึ้นของรถยนต์ไฟฟ้า อย่างไรก็ตามจากความต้องการใช้ไบโอเอทานอลที่มีแนวโน้มลดลง ดังนั้นการเพิ่มมูลค่าของไบโอเอทานอลโดยการเปลี่ยนเป็นสารเคมีชนิดอื่น เช่น อะซีโตน และเอทิลีน ซึ่งมีราคาสูงกว่าไบโอเอทานอล อีกทั้งยังสามารถนำไปใช้ในอุตสาหกรรมที่หลากหลาย และสามารถตอบสนองความต้องการที่เพิ่มขึ้นในอนาคต งานวิจัยจะเป็นการเปรียบเทียบระหว่างการผลิตอะซีโตนจากไบโอเอทานอลและการผลิตอะซีโตนและเอทิลีนจากไบโอเอทานอลโดยการเปรียบเทียบของทั้งสองกระบวนการผลิตนี้ จะเป็นการเปรียบเทียบความเป็นไปได้ทางเศรษฐศาสตร์ และ สภาวะการทำงานในกระบวนการการผลิตอะซีโตน และเอทิลีนตามลำดับ จากไบโอเอทานอล โดยใช้โปรแกรม AspenPlus V11

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Bioethanol is primarily blended with gasoline to produce "gasohol." This blend not only reduces dependence on fossil fuels but also cuts down on crude oil imports and bolsters the agricultural sector by creating a market for crops and their residues. Currently, Thailand is witnessing a growing trend towards electric vehicles (EVs). This trend is largely driven by government subsidies for domestic EV manufacturing and plans by overseas companies to establish manufacturing bases within the country. As a result, the bioethanol industry in Thailand is grappling with challenges, chief among them being the decreasing demand for its product. Nonetheless, any bioethanol surplus can be repurposed as raw material for value-added chemical compounds like acetone and ethylene. These compounds can be further refined into high-value products with a wide range of applications across various industries, potentially meeting the rising demand in the future. This study will compare the production of ethylene and acetone from bioethanol in two scenarios: the first focuses solely on acetone production, while the second encompasses both acetone and ethylene. The processes for both scenarios will be simulated using AspenPlus V11 to assess operational conditions and economic viability.

Field of Study:	Chemical Engineering	Student's Signature	....
Academic Year:	2023	Advisor's Signature	....

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INTRODUCTION

1.1Background

Bioethanol or Ethyl alcohol(C_2H_5OH) is flammable, low toxicity and colorless liquid with lower boiling point (78.5°C) melting point (-114.5°C) and density (789 kg/m³) than water. Bioethanol can be produced by the hydrolysis and sugar fermentation respectively. In Thailand, the raw materials for bioethanol production consist of molasses (58%), cassava (38%), and cane juice (4%), as shown in Table 1.

Table 1. Thai Ethanol Installed Capacity (April 2021) [1]

Feedstock	Number of plants	Installed capacity (million liters/ day)
Molasses	10	2.60
Cassava	10	2.09
Cassava & Molasses	5	1.05
Cane juice	1	0.23
Total	26	5.97

In Thailand, bioethanol is primarily used as an additive to gasoline in order to replace Methyl tert-Butyl Ether (MTBE). This blending process is known as "gasohol" and is used to increase the octane and oxygen levels in gasoline, which can help to reduce pollution emissions, decrease oversupply of agricultural produce, and decrease the need for gasoline imports. The proportion of bioethanol blended with gasoline can be 10%, 20%, or 85%, and is known as gasohol E10, E20, and E85, respectively. Since October 2012, the Thai government has mandated the use of gasohol E10 as the primary fuel in place of gasoline.

Currently, there is a growing trend of electric vehicles (EVs) in Thailand, largely due to government subsidies for domestic EV manufacturing and overseas companies

planning to establish manufacturing bases in the country, as shown in Figure 1. EVs are becoming increasingly popular due to their ability to reduce emissions, as they do not produce any tailpipe emissions, which are a major source of pollution. Additionally, they require less maintenance than traditional vehicles, as the electric engine does not require the same level of maintenance as a traditional internal combustion engine.
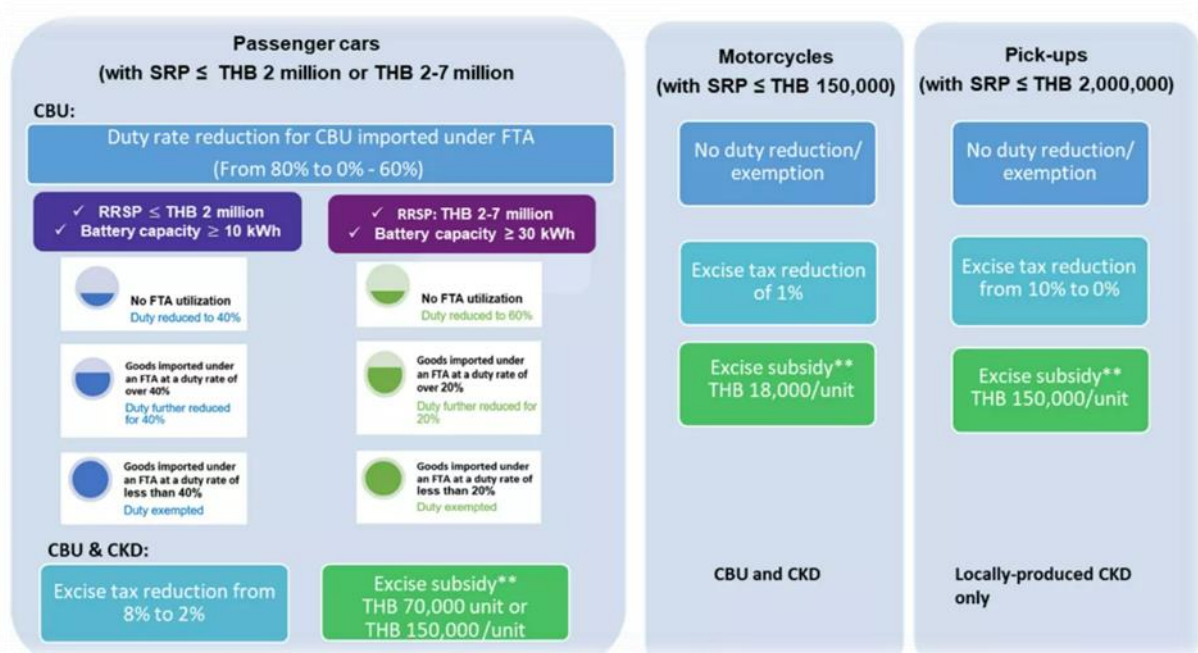
Figure 1. Government initiatives and incentives for EV adoption. [2]

From the previous paragraph, bioethanol in Thailand is currently facing a number of challenges, including a decreasing demand for the product. However, any oversupply of bioethanol can be used as raw material to produce value-added chemical compounds such as ethylene, propene, ethylene glycol, acetone, and acetic acid.

In "Decode the Future of Acetone" [3], the forecasted demand for the acetone market in Thailand shows a CAGR of 7.12%. In 2020, the acetone market demand stood at 174.77 thousand tons. The growth in demand is significantly driven by the demand for Isopropyl Alcohol and Bisphenol A, both of which are compounds

used in end-use industrial products like pharmaceuticals, adhesives, cosmetics, paints, and coatings. According to the "2023-2025 Thailand Industry Outlook" [4], the forecasted demand for ethylene is expected to increase by around 3%. Furthermore, Krungsri Research's "Thailand Industry Outlook 2023-2025" [4] states that the demand for petrochemicals, including ethylene, will increase annually by around 3%. As mentioned in the previous paragraph, acetone and ethylene are interesting chemicals as value-added products derived from bioethanol. These chemicals can be classified as bio-based chemicals, and they hold greater value than bioethanol itself.

The advantages of acetone and ethylene production from bioethanol include:

1.Sustainability: Producing acetone and ethylene from bioethanol reduces dependence on fossil fuels, such as petroleum, for their synthesis. This shift towards renewable resources promotes a sustainable and circular economy.

2.Greenhouse gas emissions: The production of bioethanol results in lower greenhouse gas emissions compared to traditional fossil fuel-derived processes. This reduction in emissions contributes to the global effort to combat climate change.

3.Energy security: By using domestically-produced bioethanol as a feedstock for acetone and ethylene, countries can reduce their reliance on imported petroleum, improving energy security and promoting self-sufficiency.

4.Rural development: Bioethanol production supports the agricultural sector by providing a market for crops and crop residues. This can lead to increased income for farmers and stimulate rural economic development.

5.Waste reduction: Converting agricultural waste and byproducts into valuable chemicals like acetone and ethylene helps to reduce waste and improve resource efficiency.

6.Biodegradable products: Acetone and ethylene derived from bioethanol are chemically identical to those produced from petroleum. However, their renewable origin can make the end products more appealing to environmentally conscious consumers who prefer biodegradable or bio-based products.

7.Technological advancements: The development of new technologies and processes to produce acetone and ethylene from bioethanol encourages innovation

and can lead to further improvements in efficiency, cost, and environmental performance. The focus of this study is on the production of acetone and ethylene as a value-added product using bioethanol.

Acetone has a wide range of applications in various industries, including:

1.Personal care industry: Acetone is used in nail polish and other cosmetic products.

2.Pharmaceutical industry: Acetone is used as a solvent and excipient.

3.Textile industry: Acetone is used as a degreaser.

4.Electronics industry: Acetone is used to clean components to achieve the maximum performance.

5.Environmental industry: Acetone is used to remove surface oil spills.

Ethylene also has a wide range of applications in various industries, including:

1.Production of polyethylene: Ethylene is the primary feedstock for the production of polyethylene, which is the world's most widely used plastic.

2.Manufacturing of other chemicals: Ethylene is used in the production of other chemicals such as ethylene oxide, ethylene glycol, and vinyl chloride.

Producing acetone and ethylene from ethanol can lead to higher-value products with versatile applications across various industries, potentially meeting increasing future demand. According to the Ministry of Energy [5], the price of ethanol is USD 1.05 per kilogram. Meanwhile, the domestic price for acetone [6] is USD 2.91 per kilogram, and for ethylene [7], it is USD 12.77 per kilogram.

In this study, acetone and ethylene production from ethanol will be simulated by using AspenPlus®V11 to analyze process simulation condition, economic feasibility and energy utilization consumption which compare in 2 cases.

1.2 Research Objectives

The purpose of this study is to design and simulate the process of acetone and ethylene production from ethanol by using AspenPlus®V11 to analyze the process conditions, economic feasibility, and energy evaluation for two cases, one with ZnO catalyst and ZnO-CaO catalysts, while keeping the operating conditions the same.

1.3 Research scopes

1.3.1 To simulate the process of acetone and ethylene production from bioethanol using Aspen Plus® V11, and analyze the results for both production cases.

1.3.2 To assess the economic feasibility of acetone and ethylene production from bioethanol using Aspen Plus® V11, and compare the results for the two production cases.

1.3.3 To analyze the energy consumption and utilization in acetone and ethylene production from bioethanol using Aspen Plus® V11, comparing the results for both production cases.

1.3.4 To develop a simulation model for ethylene and acetone production from bioethanol that incorporates heat exchanger networks, aiming to optimize energy efficiency.

By achieving these research scopes, the aim to identify which catalyst yields better results and contribute to the development of sustainable and cost-effective acetone and ethylene production methods.

1.4 Research benefits

1.4.1 The ability to scale up the process from laboratory to commercial scale, which would enable large-scale production of acetone and ethylene from ethanol.

1.4.2 A better understanding of the unit operations and operating conditions necessary to produce acetone and ethylene from ethanol.

1.4.3 An assessment of the feasibility of the process from both economic and energy utilization perspectives.

1.5 Research methodology

Studying acetone and ethylene production from ethanol by using catalytic reaction from literature review. (Lab scale)

Design the process from lab scale to commercial scale.

Simulate the process from designing commercial scale by using AspenPlus®

Economic analysis by using AspenPlus®

No

Yes

Discussion the results and conclusion of the process.
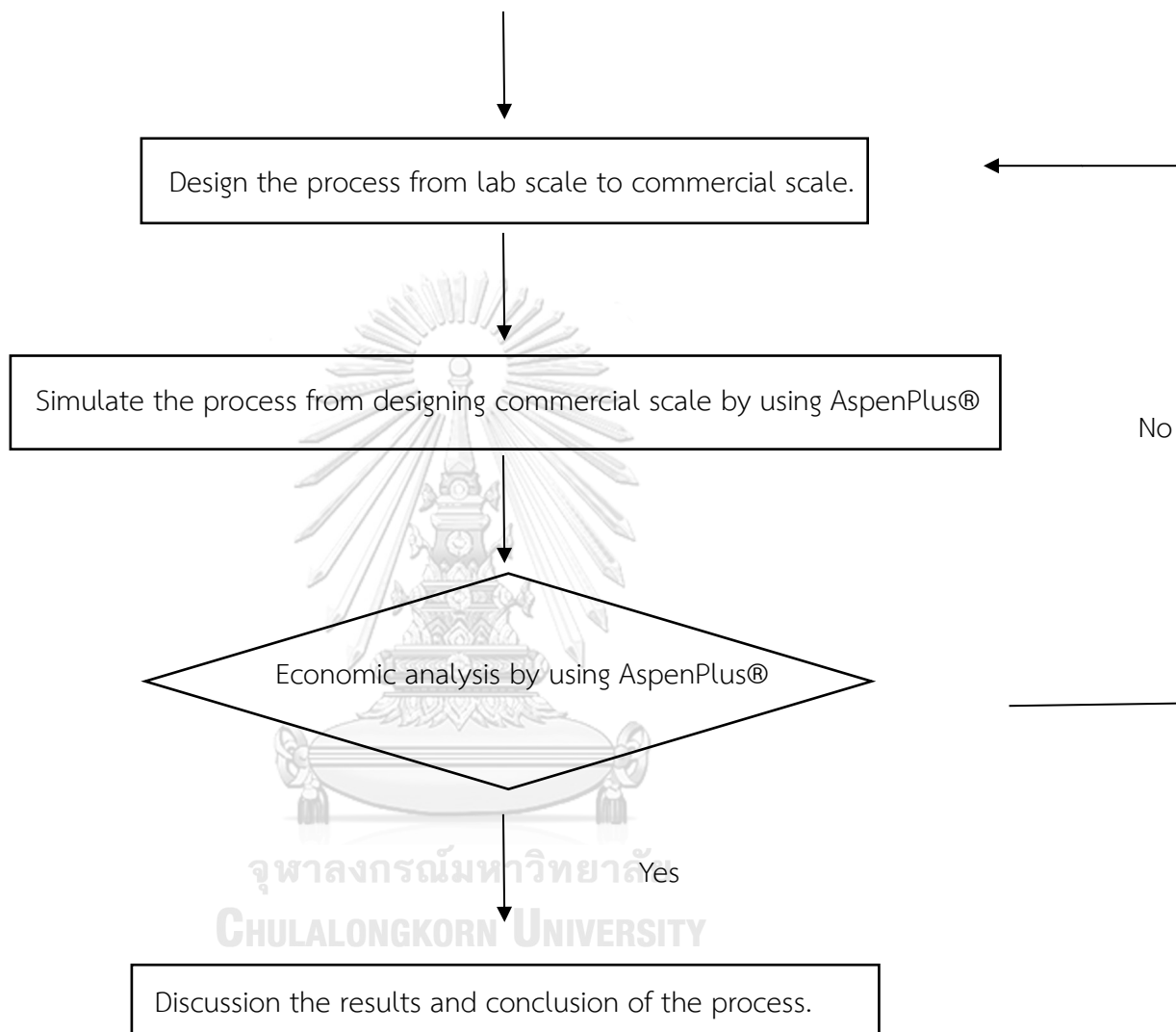
CHAPTER 2

THEORY AND LITERATURE REVIEW

This chapter offers an overview of the theoretical foundation pertinent to this research. It encompasses descriptions of the properties of the compounds in focus—acetone, ethylene, and ethanol. The chapter elucidates the reaction mechanism for acetone and ethylene production from ethanol, reviews relevant literature on the production of acetone and ethylene from ethanol, and details the separation process used in the simulations for this study.

2.1 THEORY

2.1.1 Ethanol

Ethanol, also known as ethyl alcohol, is a clear, colorless, highly volatile, and highly flammable chemical compound that easily dissolves in water, as shown in Table 2. Its chemical formula is C_2H_5OH (see Figure 2). It can be produced through the fermentation of agricultural produce, resulting in a product called ethanol, or through the hydration of ethylene.
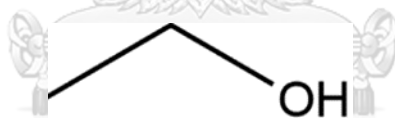
Figure 2 Chemical Structure of Ethanol [8]

Table 2 Physical and Chemical properties of ethanol [9]

Properties	Value
Physical State	Clear liquid
Appearance	Colorless
Odor	Mild, pleasant
Viscosity	1.20 cP @20°C
Boiling Point	78°C
Freezing Point	-114.1°C
Solubility	Miscible
Specific Gravity	0.79 @20°C
Molecular Weight	46.0414

There are many chemicals produced using ethanol as a precursor for value-added
products, such as ethylene, BTX (an approximate stoichiometry of the global supply
of benzene, toluene, and xylenes), isobutene, propene, and acetone, as shown in
Figure 3.
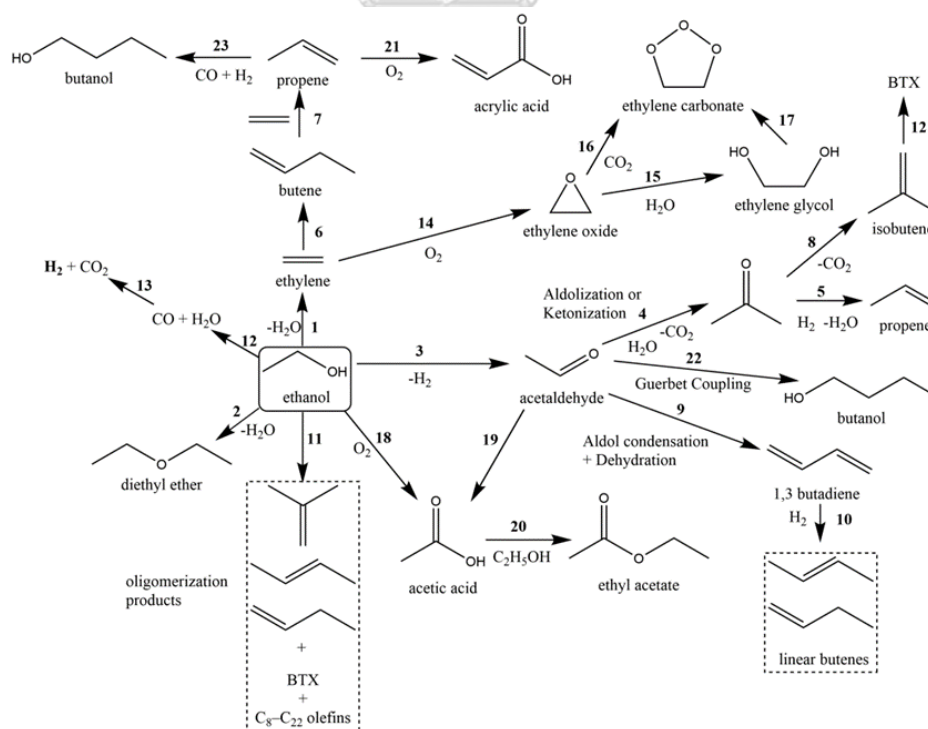
Figure 3 Pathways of value-added ethanol [8]

2.1.2   Acetone

Acetone, also known as propanone, is a clear, colorless, highly volatile, and highly flammable chemical compound that easily dissolves in water, as shown in Table 3. Its chemical formula is $(CH_3)_2CO$ (see Figure 4). The most common production method for acetone is through co-production in the cumene process.
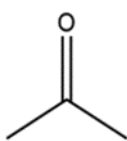
Figure 4 Chemical Structure of Acetone [8]

Table 3 Physical and Chemical properties of acetone [10], [11]

Properties	Value
Physical State	Liquid
Appearance	Colorless
Odor	Pungent
Viscosity	0.36 cP @20°C
Boiling Point	56.08°C
Freezing Point	-94.7°C
Solubility	Miscible
Specific Gravity	0.7845 @20°C
Molecular Weight	58.079

In addition to its use in the chemicals, pharmaceutical, and textile industries, acetone is also commonly used as a cleaning agent, nail polish remover, and degreaser. The demand for acetone in these applications is driven by the consumer market.

Nowadays, bioacetone has been produced through ABE (acetone-butanol-ethanol) fermentation, using carbohydrates such as starches and sugars and Clostridium acetobutylicum or other related bacteria. Companies in Scotland (Celtic Renewables), the US (Gevo), India (Godavari Biorefineries Ltd.), and China (Godavari Biorefineries Ltd.) are involved in bioacetone production.[12]

2.1.3 Ethylene

Ethylene, also known as ethene, is a colorless gas at room temperature and has a lower density than air, as shown in Table 5. It is highly flammable, and its chemical formula is C_2H_4 (see Figure 5). The most common method of producing ethylene is through a process called steam cracking, which involves breaking down hydrocarbons using high temperature and pressure.
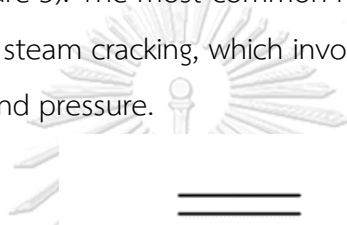
Figure 5 Chemical Structure of Ethylene [13]

Table 4 Physical and Chemical properties of ethylene [14 ,15]

Properties	Value
Physical State	Gas
Appearance	Colorless
Odor	Sweet and musky
Viscosity	0.0103 cP @25°C
Boiling Point	-103.7°C
Specific Gravity	0.978 @25°C
Molecular Weight	28.054

2.1.4 The reaction mechanism to produce acetone and ethylene from ethanol.

There are 2 pathways to produce acetone from ethanol with   thermocatalytic reactions.

The first pathway of acetone production from ethanol called "ketonization". Ketonization is a chemical process that converts a primary or secondary alcohol into a ketone through the use of an oxidizing agent, such as concentrated sulfuric acid. The reaction typically involves the addition of the oxidizing agent to the alcohol,

which leads to the formation of an intermediate aldehyde and then to a ketone. Ketonization is used in the production of certain chemicals, such as acetone, and is an important step in the industrial synthesis of certain compounds.

Ethanol is dehydrogenation to acetaldehyde and hydrogen.[16]

$$CH_3CH_2OH \longrightarrow CH_3CHO + H_2 \tag{2.1}$$
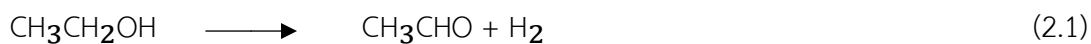
Ethanol is dehydration to ethylene and water. [16]

$$CH_3CH_2OH \longrightarrow C_2H_4 + H_2O \tag{2.2}$$

Acetaldehyde is oxidation to acetic acid. [16]

$$CH_3CHO + H_2O \longrightarrow CH_3COOH + H_2 \tag{2.3}$$
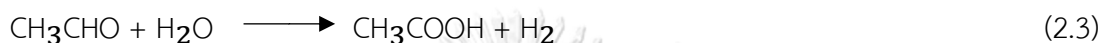
Acetic acid is ketonization to acetone. [16]

$$2CH_3COOH \longrightarrow CH_3COCH_3 + CO_2 + H_2O \tag{2.4}$$
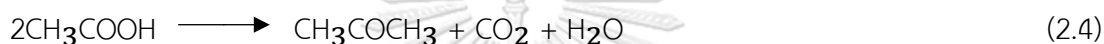
The second pathway of acetone production from ethanol called "aldol addition" Aldol addition is a chemical reaction that results in the formation of a new carbon-carbon bond between two aldehyde or ketone molecules. This reaction occurs through the nucleophilic addition of an enolate ion to an aldehyde or ketone molecule, resulting in the formation of a β-hydroxy aldehyde or ketone. The reaction is called an aldol addition because it leads to the formation of an aldol, which is a molecule that contains both an aldehyde and an alcohol functional group. Aldol additions are widely used in organic synthesis, as they provide a convenient way to form carbon-carbon bonds and construct complex molecules.

Ethanol is dehydrogenation to acetaldehyde and hydrogen. [16]

$$CH_3CH_2OH \longrightarrow CH_3CHO + H_2 \tag{2.5}$$
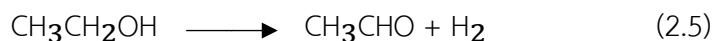
Ethanol is dehydration to ethylene. [16]

$$CH_3CH_2OH \longrightarrow C_2H_4 + H_2O \tag{2.6}$$
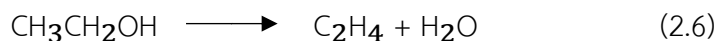
Acetaldehyde is aldol addition to 3-hydroxybutanal as following. [16]

$$CH_3CHO + CH_3CH_2OH \longrightarrow CH_3CH(OH)CH_2CHO + H_2 \tag{2.7}$$
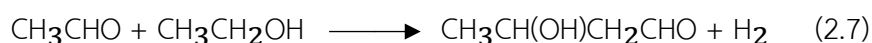
3-hydroxybutanal is decarboxylation and dehydrogenation to acetone. [16]

$$CH_3CH(OH)CH_2CHO + O\,[lattice] \longrightarrow CH_3COCH_3 + CO_2 + H_2 \tag{2.8}$$
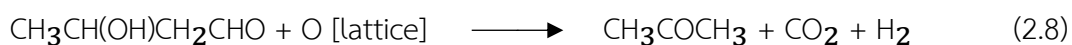
From equation (2.4) and (2.8) show the acetone production by the difference way of reaction, the reactant and by-products as show in table5.

Table 5 The difference between acetone and ethylene production mechanism.

Details	Ketonization	Aldol Addition
Reactants	CH_3CH_2OH, H_2O	CH_3CH_2OH
By-products	CO_2, H_2	CO_2, H_2
Undesired products	C_2H_4	C_2H_4

2.2 Literature review

2.2.1 Reaction and Catalysts related to acetone and ethylene production.

From the section 2.1.3 the diversity of catalyst and operating conditions to produce acetone from ethanol as table 6

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Table 6 Catalysts and operating conditions to produce acetone and ethylene from ethanol.

Item	Catalyst	Operating Conditions	%Conversion of ethanol	%Yield of acetone	%Yield of ethylene	Mechanism	Remark	Ref.
1.	ZnO-CaO (9:1)	400°C 1 atm	100%	91%	9%	Ketonization		[17]
2.	ZnO	400°C 1 atm	98.6%	40%	50%	Ketonization		[17]
3.	CZA-ZrO$_2$ (1:2)	400°C 1 atm	88%	43.7%	-	Ketonization		[18]
4.	ZnFe$_2$O$_4$	400°C	100%	94%	-	Ketonization	catalyst life < 24 hrs.	[19]
5.	CZA-CeZr	-	74%	60%	5%	Ketonization		[20]
6.	Cu/La$_2$Zr$_2$O$_7$	400°C 1 atm	62%	72%	-	Ketonization	catalyst life < 200 mins.	[21]
7.	La$_{0.7}$Sr$_{0.3}$MnO$_3$	476°C 1 atm	99%	80%	-	Aldol Addition		[21]
8.	20 mol% CuO/CeO$_2$ 0.5 g	300°C 1 atm	95.7%	35.9%	-	Aldol Addition		[22]

Item	Catalyst	Operating Conditions	%Conversion of ethanol	%Yield of acetone	%Yield of ethylene	Mechanism	Remark	Ref.
9.	ZnO-CoO/Al$_2$O$_3$	400°C 1 atm	97%	45%	Not specify	Aldol Addition	Does not specify all the byproducts that occurred.	[23]
10.	Fe$_2$O$_3$: CaO	450°C	90%	52%	Not specify	Not Specify	Does not specify all the byproducts that occurred, and catalyst deactivate rapidly.	[24]
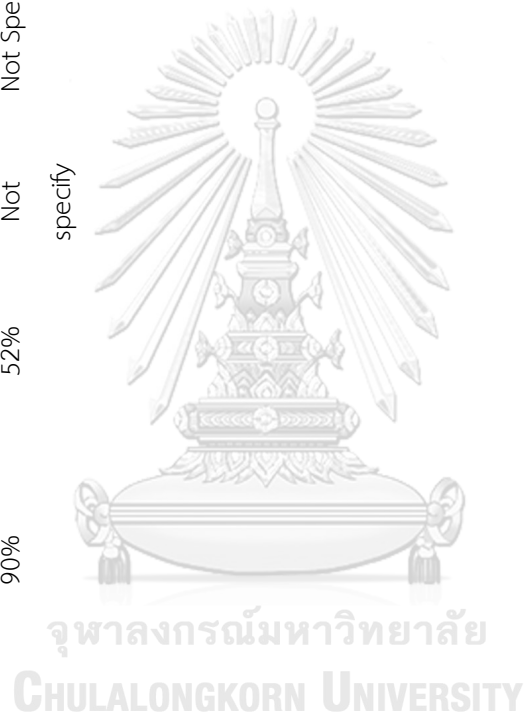
From Table 6, the catalyst with the highest ethanol conversion (100%) consists of ZnO-CaO and $ZnFe_2O_4$. However, the catalyst life of $ZnFe_2O_4$ is less than 24 hours, making the ZnO-CaO catalyst more desirable for achieving 100% ethanol conversion to produce acetone. The next most efficient catalyst is $La_{0.7}Sr_{0.3}MnO_3$ with an ethanol conversion of 99%. However, this catalyst is not commercially available and must be synthesized. Lanthanum and Strontium, which are more costly than other more abundant elements, make up its composition. Furthermore, the acetone yield of ZnO-CaO is higher than that of the $La_{0.7}Sr_{0.3}MnO_3$ catalyst, making it unsuitable for comparison with the ZnO-CaO catalyst in acetone production. The next most efficient catalyst is ZnO, with an ethanol conversion of 98.6% and acetone and ethylene yields of 40% and 50%, respectively. This catalyst can be compared to the ZnO-CaO catalyst, as both are commercially available and easily supplied. A comparison of the techno-economic aspects of these catalysts can help determine which one is more cost-effective for large-scale production of acetone and ethylene from ethanol.

The ZnO-CaO and ZnO catalysts are compared in two cases: the first case involves the use of ZnO-CaO catalyst to produce acetone from ethanol, while the second case employs ZnO catalyst to produce both acetone and ethylene from ethanol. A literature review reveals that both catalysts have been synthesized, and Temperature-Programmed Decomposition (TPD) has been used to analyze the effect of calcination temperature on the activity and yield of ethanol conversion. Ethanol and water, at concentrations of 36 wt% and 64 wt% respectively, were fed into a fixed-bed reactor at atmospheric pressure. The reaction temperature was set at 400°C with a residence time of 0.435 seconds. The reactor was wrapped with an iron sheet to prevent temperature fluctuations. The reactants and products from the reactor were analyzed using gas chromatography.

2.2.2 Methods for Separating Troublesome By-products.

In the second case study, which delves into the production of acetone and ethylene from ethanol, a variety of conventional technologies are employed to purify the gas phase. These technologies encompass adsorption, absorption-stripping, membrane separation, and cryogenic distillation.

2.2.2.1 Adsorption technology

Adsorption is a process where a liquid or gas, termed the 'adsorbate', accumulates on the surface of a solid, which is referred to as the 'adsorbent'. This accumulation arises due to diverse forces or interactions, such as Van der Waals forces, electrostatic forces, covalent bonds, or even specific chemical reactions. The kind of interaction depends on the type of adsorption, which can be either physical or chemical. [26]

Physical adsorption

Physical adsorption is typified by forces or interactions like Van der Waals or electrostatic forces. This process is reversible and highly sensitive to temperature changes. Contrary to some processes, physical adsorption doesn't necessitate activation energy and can result in the creation of multiple layers on the adsorbent surface. It demonstrates the highest efficacy at low temperatures and elevated pressures. [26]

Chemical adsorption

Also known as chemisorption, chemical adsorption is driven by forces or interactions such as covalent bonds or specific chemical reactions, culminating in the creation of surface compounds. This process is irreversible, necessitates activation energy, and results in the formation of a singular monolayer on the adsorbent's surface. It is most effective at heightened temperatures. [26,27]

Criteria to use Adsorption

While distillation and air stripping stand as the primary techniques for separating components in liquid phases based on relative volatility, adsorption becomes a favored method under distinct conditions. These include scenarios where the relative volatility between pivotal components is minimal, the chief component in the feed is of diminished value, and the desired product is present in sparse concentrations. Moreover, situations where the boiling points of components overlap or when low temperatures and high pressures are vital make adsorption a preferred choice. Additionally, if there's potential heat-induced damage or alteration to components in the feed, or challenges like chemical corrosion, unwelcome chemical reactions, or situations prompting equipment fouling arise, adsorption becomes an attractive remedy. Under the right circumstances, adsorption proves to be cost-efficient, especially for mid-level throughputs and when there isn't a strict demand for ultra-high purity. If the feed gas is inherently pressurized, adsorption's cost benefits amplify significantly. [26]

CO$_2$ Adsorption

Drawing from the study "CO$_2$ adsorption by swing technologies and challenges on industrialization" [28], various swing adsorption techniques including pressure swing adsorption (PSA), temperature swing adsorption (TSA), vacuum pressure swing adsorption (VPSA), and electrical thermal swing adsorption (ETSA) are utilized for CO$_2$ adsorption. In PSA, CO$_2$ is primarily adsorbed onto a solid adsorbent under high pressure. This adsorption is then reversed by decreasing the pressure, typically to atmospheric levels. In TSA, the adsorbent's ability to capture CO$_2$ is temperature-dependent. It exhibits greater adsorption at elevated temperatures, whereas other gases like N$_2$ consistently showcase low adsorption capacities across temperature ranges. In TSA, the adsorbent's ability to capture CO$_2$ is temperature-dependent. It exhibits greater adsorption at elevated temperatures, whereas other gases like N$_2$

consistently showcase low adsorption capacities across temperature ranges. VPSA, alternatively known as Vacuum Swing Adsorption (VSA), typically operates at higher feed temperatures during the adsorption phase and undergoes recovery at or below atmospheric pressures. ETSA, as introduced by Fabuss and Dubois, serves as an enhancement to the TSA method, especially when deploying hot gas. In contrast to TSA, which employs hot gas as its heat source, ETSA capitalizes on the Joule effect by channeling electricity through the adsorption column. For this process to be effective, the adsorbent must possess electrical conductivity. By applying a low-voltage electric current, CO_2 is released from the adsorbent. Preliminary assessments suggest that ETSA may offer a more cost-effective strategy for CO_2 capture than its traditional counterparts. [28]

2.2.2.2 Absorption and Stripping technology

Absorption and stripping are opposite processes in which gases or contaminants are transferred between the liquid and gas phases. While absorption entails the solubilization of a gas component into a liquid, stripping involves moving a contaminant from a liquid to a gas phase. Absorption can be classified into two types: physical absorption and chemical absorption. [26]

Physical Absorption

Physical absorption is primarily based on solubility differences. It involves the removal of a gaseous component due to its differential solubility between the gas and liquid phases. There isn't a chemical reaction between the gas and the solvent; instead, the gas simply dissolves into the solvent. [26]

Chemical Absorption

Chemical absorption requires a chemical reaction between the gas to be removed and a compound present in the liquid solvent. As a result of this reaction, the gas remains in solution. [26]

CO_2 Absorption

In physical absorption, the solubility of CO_2 in a solvent increase under high pressure within a gas-liquid contactor. When this solvent is then moved to a low-pressure flash tank, CO_2 bubbles form and release. This action initiates the desorption process, eventually reaching equilibrium where the liquid is no longer supersaturated with CO_2. [29] Conversely, in chemical absorption, CO_2-rich flue gas enters at the bottom of the absorber, flowing counter-currently to the lean liquid solvent. As they interact, chemical reactions take place between CO_2 and the solvent. The resulting purified exhaust gas exits from the top of the column, being directed to the stack. [30]

2.2.2.3 Membrane Technology

A membrane is a semi-permeable barrier between two phases, selectively restricting molecule movement. While the barrier can be solid, liquid, or gas, its selectivity ensures separation. Separation mechanisms include size exclusion, differing diffusion rates, electrical charge, and solubility variations. Unlike methods relying on equilibrium, membrane separation is driven by an external force.[26]

For the separation of gas mixtures where both the feed and permeate streams are in the gas phase, the driving force is the difference in partial pressure. The membrane used is usually a dense film, and the transport method is sorption–diffusion. For

polymer materials below their glass transition temperature, the "dual-mode" transport model is commonly applied.[26]

2.2.2.4 Cryogenic distillation technology

Cryogenic distillation separates components from a gas stream at extremely low temperatures and under high pressure based on their boiling points or relative volatility. Components with lower boiling points are collected at the top, while those with higher boiling points settle at the bottom as liquid. The column's efficiency is influenced by its operating temperature and pressure. The column usually operates in a two-phase region, with liquid flowing downwards and vapor rising counter-currently. The separation's mass transfer primarily occurs during the vapor-liquid in

Acetone and ethylene are produced as described in the second case. The chemical reactions mechanism is detailed from equation (2.1) to (2.4). From these equations, it is evident that CO_2 and H_2 are by-products. To purify ethylene (C_2H_4), both reactive absorption and cryogenic distillation are considered. Reactive absorption (or chemical absorption) is favored for CO_2 separation for several reasons:

1.Cryogenic Distillation operates under high pressure and low temperatures, leading to increased utility costs

2.Membranes, while a potential solution for CO_2 capture, face challenges in performance, real-world applicability, economic viability, integration, and necessitate enhanced collaboration between power plants and membrane developers.[33]

3.Adsorption is effective only at low CO_2 concentrations, and the sorbent utilized is not optimal for CO_2 capture.[34]

To separate CO_2, the Reactive Absorption-Stripping method is employed. During the absorption stage, a reaction between CO_2 and the MEA (Monoethanolamine) solution facilitates the transfer of CO_2 from the gas phase to the liquid phase.

Conversely, in the stripping stage, CO_2 is released from the MEA solution. The reaction mechanism between CO_2 and MEA is presented in equations (2.9) to (2.13).[30]

Chemical Reactions in reactive absorption

$$2H_2O \rightleftharpoons H_3O^+ + OH^- \tag{2.9}$$

$$MEA^+ + H_2O \rightleftharpoons H_3O^+ + MEA \tag{2.10}$$

$$HCO_3^- + H_2O \rightleftharpoons H_3O^+ + CO_3^{2-} \tag{2.11}$$

$$CO_2 + MEA + H_2O \rightleftharpoons MEACOO^- + H_3O^+ \tag{2.12}$$

$$CO_2 + OH^- \rightleftharpoons HCO_3^- \tag{2.13}$$
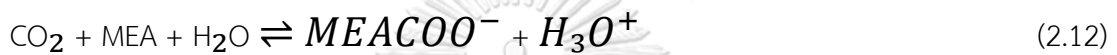
Equations (2.9) to (2.11) describe the equilibrium reactions from the reactive absorption. The coefficients of the equilibrium constants for these reactions are presented in equation (2.14) and can be found in Table 7. On the other hand, the reversible kinetic reactions are outlined in equations (2.12) and (2.13), with their respective kinetic parameters detailed in Table 8.

The temperature dependence equation for reaction (2.9) to (2.11).[35]

$$K_i = \exp\left(A + \frac{B}{T} + C \ln(T) + DT\right) \tag{2.14}$$

Table 7 Coefficients of equilibrium constants of equation (2.14) [35]

Equation	K_i	A	B	C	D	Temperature(K)
(2.9)	$K_{2.9}$	132.899	-13445.9	-22.4773	0	273-498
(2.10)	$K_{2.10}$	2.1211	-8189.38	0	-0.007484	273-323
(2.11)	$K_{2.11}$	216.049	-12431.7	-35.4819	0	273.498

Table 8 kinetic parameter [30]

Equation	Forward reaction		Reverse reaction		Order of rate law expression
	k^0_{fj} [kmol/(m^3 s)]	E_j [cal/mol]	k°_{fj} [kmol/(m^3 s)]	E_j [cal/mol]	
(2.12)	9.77(10^10)	9855.8	3.23(10^19)	15655	2nd
(2.13)	4.32(10^13)	13249	2.38(10^17)	29451	2nd

Cryogenic distillation is utilized to purify ethylene. This method can achieve an ethylene purity of over 99%. It is effective in separating gas mixtures and can be employed to purify ethylene across various scales.[36]

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CHULALONGKORN UNIVERSITY

CHAPTER 3

Methodology

This chapter provides an overview of the study's design scope, detailing the feed preparation process and presenting a preliminary design with a block flow diagram. It includes a thorough process description, complete with a process flow diagram, and conducts an economic analysis. This analysis encompasses cost assumptions for raw materials, catalysts, and utilities, as well as product valuations, all essential for calculating economic feasibility. Additionally, it introduces an economic index to gauge the potential for investment.

3.1 Design Scope

In chapter 2, the operating conditions for the study were set at 400°C and 1 atm, and the ZnO-CaO catalyst and ZnO catalyst were chosen for techno-economic comparison. The ZnO-CaO catalyst with a 9:1 mole ratio demonstrated 100% ethanol conversion, 91% acetone yield, and 9% ethylene yield. In contrast, the ZnO catalyst achieved 98.6% ethanol conversion, 40% acetone yield, 50% ethylene yield, and 8% acetaldehyde yield.

Table 9 Catalysts, conversion of ethanol and yield of product with 400°C and 1 atm operations.

Item	Catalyst	Conversion of ethanol	Yield of product
1.	ZnO-CaO	1	0.91 of acetone and 0.09 of ethylene
2.	ZnO	0.986	0.4 of acetone, 0.5 of ethylene and 0.08 of acetaldehyde

From table 6. The definition of parameters can explain for using in mass balance as equation (3.1) and (3.2)

Conversion = <u>moles of ethanol reacted</u>   (3.1)

                          moles of ethanol feed

Yield = <u>moles of ethanol convert to product</u>   (3.2)

                          moles of ethanol feed

3.2 Feed Preparation

To produce acetone and ethylene from ethanol, the feed stream consists of ethanol and water obtained from an outsource that contains 95% ethanol. Before passing to the reactor, the feed stream is adjusted to a composition of 36 wt% ethanol and 64 wt% water. To study the techno-economics and feasibility of the process, two cases were considered. In the first case, acetone production from ethanol was studied using a ZnO-CaO catalyst to produce 50,000 tons/year of acetone. The feed stream to the reactor for this case was 242,095.07 tons/year, with a composition of 36 wt% ethanol and 64 wt% water. In the second case, both ethanol and ethylene were produced. To facilitate comparison of the two cases, the feed stream to the reactor was held constant at 242,095.07 tons/year, which corresponds to the same feed composition of 36 wt% ethanol and 64 wt% water.

3.3 Preliminary Design

The conceptual design for producing acetone and ethylene from ethanol was studied for two cases including:

3.3.1 Feed preparation system

The fresh feed stream of 95% ethanol and any accompanying water is stored at ambient temperature and pressure (1 atm and 30°C). This stream is then combined with the recycle stream and fed to the reactor, resulting in a mass fraction of 0.36 ethanol and 0.64 water. The annual quantities of ethanol and water involved in this process are 87,154.23 tons/year and 154,940.84 tons/year, respectively.

3.3.2 Reactor system

Following the feed preparation system, both the ethanol and water streams are introduced into the reactor, where they undergo the critical ketonization reactions outlined in equations (2.1) to (2.4). The reactor is operated at 400°C and 1 atm, and two different catalysts are used: ZnO-CaO in the first case and ZnO in the second. The specific choice of operating conditions and catalysts are based on their ability to promote the desired reaction pathways and achieve optimal conversion rates.

After the reactor system, all of the chemicals, including both products and reactants, are in the form of gas or vapor. When they pass through the phase separation system, the gas phase containing ethylene, CO_2, and H_2 will separate into the gas phase, while the vapor phase containing acetone and water (in the first case) or acetone, water, acetaldehyde, and unreacted ethanol (in the second case) will separate into the liquid phase.

3.3.4 Gas separation system

In the second case, the vapor phase from the phase separation system will separate into the liquid phase, while the gas phase will pass through a gas separation system to separate the ethylene.

3.3.5 Liquid separation system

To purify and separate acetone, the liquid phase from the phase separation system will pass through a liquid separation system, which will separate acetone from water (in the first case) or from unreacted ethanol (in the second case, assuming an ethanol conversion of 0.986), as well as from water and acetaldehyde.

3.3.6 Recycle system

Water and ethanol are the reactants in this process. To reduce the amount of fresh feed water required in the first case, the water from the liquid separation system and the ethanol and water from the liquid separation system in the second case will pass through a recycle system, which allows for the reuse of these reactants
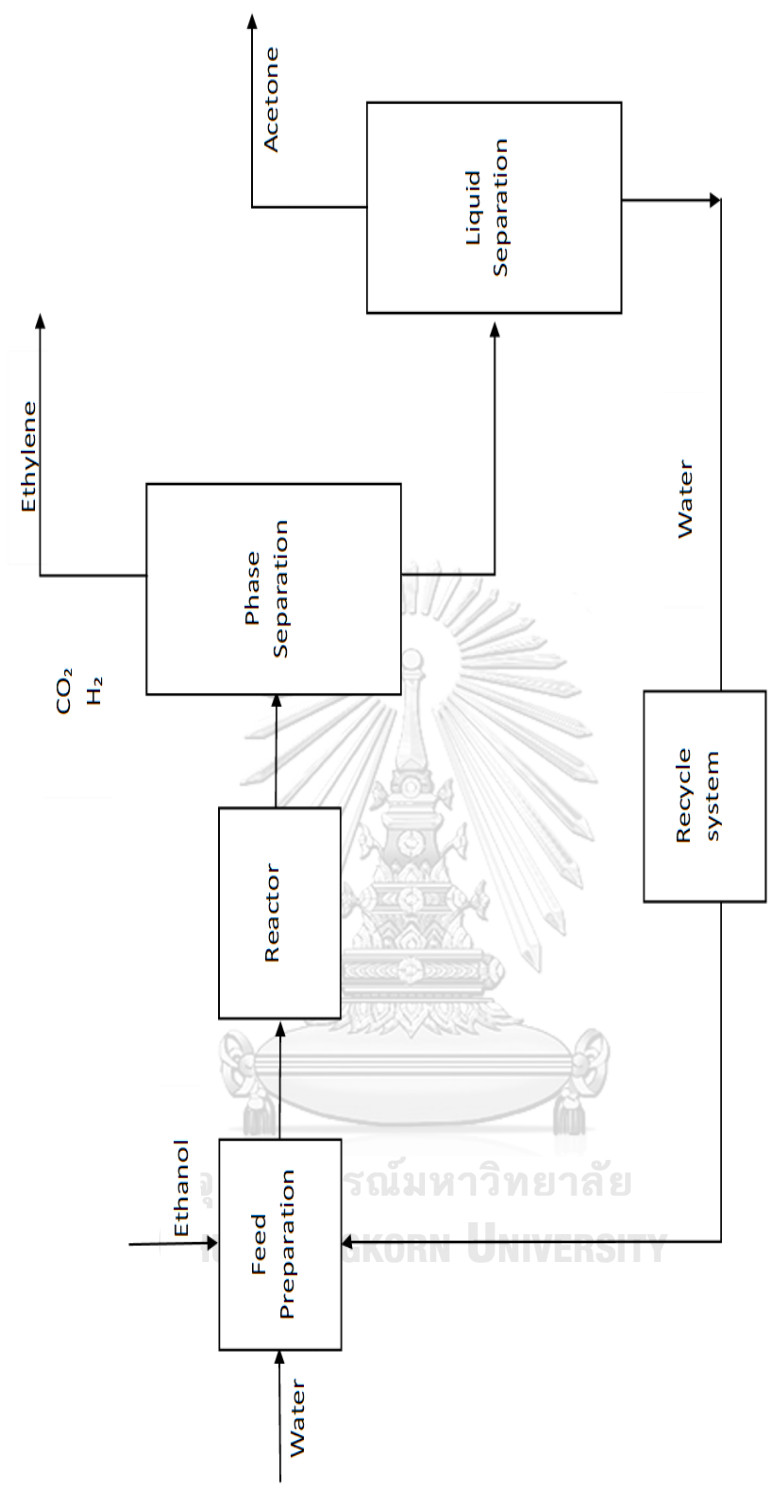
Figure 6 Block flow diagram of acetone production from ethanol by using ZnO-CaO catalyst.
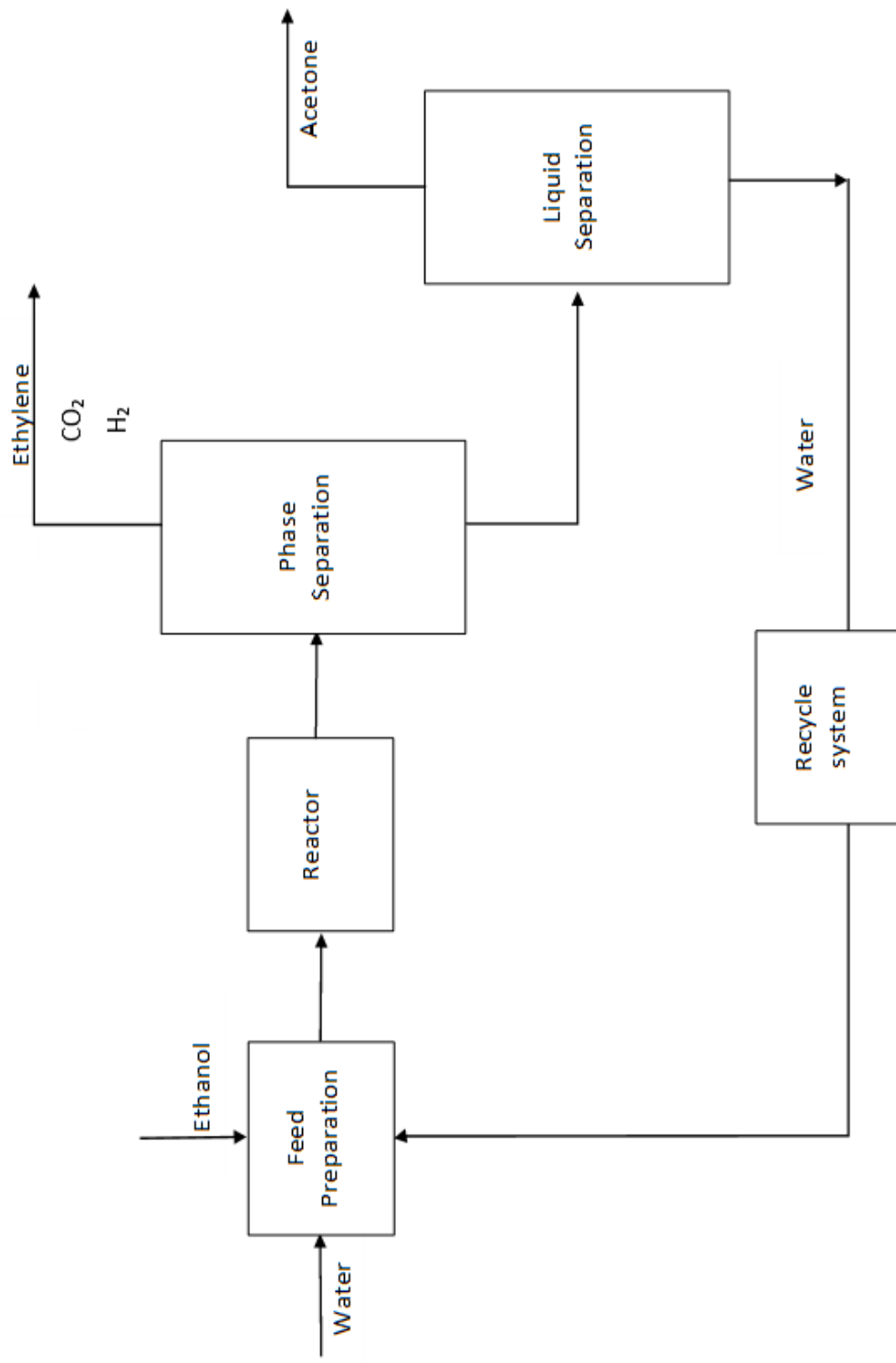
Figure 7 Block flow diagram of acetone and ethylene production from ethanol by using ZnO catalyst.

3.4 Process Description

In this work, there are two cases. The first case involves acetone production from ethanol using a ZnO-CaO catalyst, while the second case involves the production of acetone and ethylene from ethanol using a ZnO catalyst. Both of these cases were simulated using the Aspen Plus V11 program for this research.

Figure 8 depicts the process of synthesizing acetone from bioethanol using a ZnO-CaO catalyst. A fresh ethanol feed (ETOH-F) with a 95% concentration, water (WATER-F), and a recycle stream (RECYCLE) are merged in mixer M-1 to create a consistent stream. Annually, this stream consists of 87,154.23 tons of ethanol and 154,940.84 tons of water, and it leads to the production of 50,000 tons of acetone. Prior to entry into the reactors R-1, R-2, and R-3, the mixture is progressively preheated in heat exchangers E-1 and E-2 to a temperature of 400°C. The resulting mixture, now containing acetone, water, ethylene, CO_2, and H_2, is unified again in mixer M-2. This mixture is then passed through compressed in compressor C-1 to increase the pressure. It is then channeled through heat exchangers E-3 and E-4 for cooling down the stream. Once it exits heat exchanger E-4 the product stream is conveyed to phase separator S-1, which segregates the vapor and liquid phases. The vapor phase is removed (PURGE-1), while the liquid phase, containing acetone, water, and trace amounts of ethylene, CO_2, and H_2, is collected. This liquid is then sent through valve V-1 to decrease its pressure and subsequently fed into the distillation column S-2. From the top of the column, minor quantities of ethylene, CO_2, and H_2 are eliminated (PURGE-2), and the acetone is refined to a desired purity of 95%. Water is drawn from the bottom of the distillation column and is pressure-reduced via a valve before being looped back into the process as part of the recycle stream.

Figures 9 to 12 illustrate the process of producing acetone and ethylene from bioethanol using a ZnO catalyst. The ethanol feed (ETOH-F) at a 95% concentration is mixed with water (WATER-F) and a recycle stream (RECYCLE1) in mixer M-1, creating a uniform stream. This approach is consistent with the process depicted in Figure 6 (Case I), which uses a ZnO-CaO catalyst, allowing for direct comparisons of feed

amounts for investment feasibility studies. Before entering reactors R-1, R-2, R-3 and R-4, the mixture is sequentially preheated in heat exchangers E-1 through E-2 until it reaches 400°C. The post-reaction output—including ethanol, water, acetone, acetaldehyde, ethylene, CO_2, and H_2—is consolidated in mixer M-2. This product stream is then compressed in compressor C-1, which increases the pressure. The pressurized vapor then cools by passing through heat exchangers E-3, which facilitates a heat exchange—cooling the product stream while concurrently warming the cooling water stream and pass through phase separator S-1. The heavier bottom stream from S-1 is pressurized by pump P-3 before moving on to mixer M-4. The lighter top stream (vapor phase) from S-1 is directed into the reactive absorption column (ABSORP). In mixer M-3, a 90% monoethanolamine (MEA) solution (MEA-F), additional water (WATER-F2), and another recycle stream (RECYCLE2) are combined and introduced at the top of ABSORP in a liquid phase. The vapor phase from S-1 enters the bottom of ABSORP, where the CO_2 reacts with MEA, separating from the vapor phase. After absorption, the CO_2-depleted bottom stream is pressurized by pump P-1 and sent to the stripping column (STRIPPER) for MEA regeneration. The stream exiting STRIPPER is further pressurized by pump P-2 and rerouted through heat exchanger E-5, then proceeds to phase separator S-12, where the liquid phase is drained from the bottom, and the vapor phase is cooled in heat exchangers E-6 with cooling water before passing through mixer M-3 as RECYCLE2, which contains water and MEA. At the top of ABSORP, trace amounts of CO_2 are compressed by C-2 and cooled in E-4 with cooling water before entering to phase separator S-2. The output goes to phase separator S-2, where the liquid phase joins the flow in mixer M-4, and the vapor phase enters distillation column S-3. In S-3, the heavier bottom stream merges with the contents from M-4, while the lighter top stream is compressed by C-3, cooled in E-7 with chilled water, and then directed to phase separator S-4. The liquid phase from S-4 is depressurized through valve V-1 and routed to mixer M-4. Concurrently, the lighter top output is pressurized by C-4 and conveyed to cryogenic distillation columns S-5 to S-7, where ethylene is purified to 99% purity. The stream from mixer M-4 enters distillation columns S-8 to S-10 to concentrate the acetone to

95%. Finally, the heavy stream from the bottom of S-10 is depressurized via valve V-3 and processed through phase separator S-11. The vapor phase from S-11 is purged, and the liquid phase is recycled back to mixer M-1.
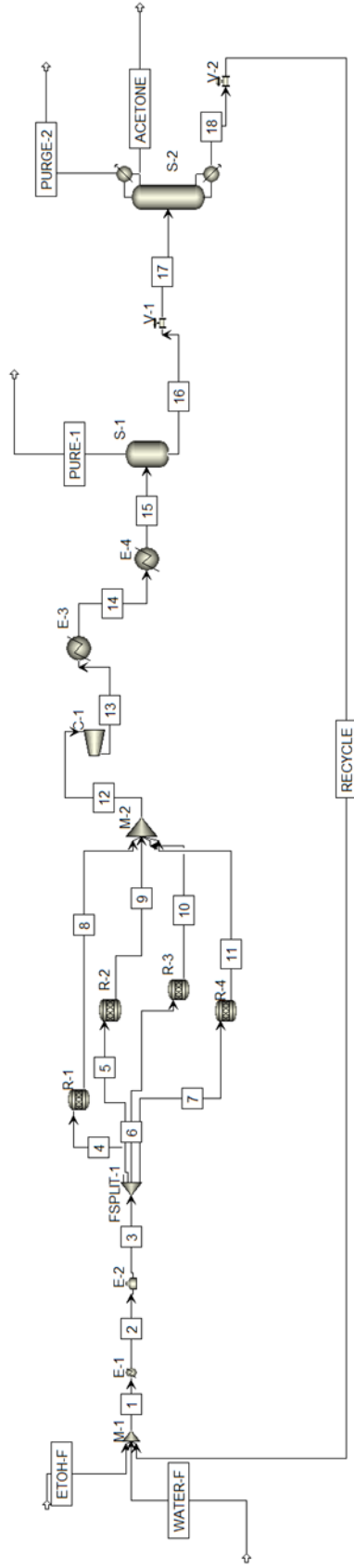
Figure 8 Process flow diagram of acetone production from bioethanol by using a ZnO-CaO catalyst.
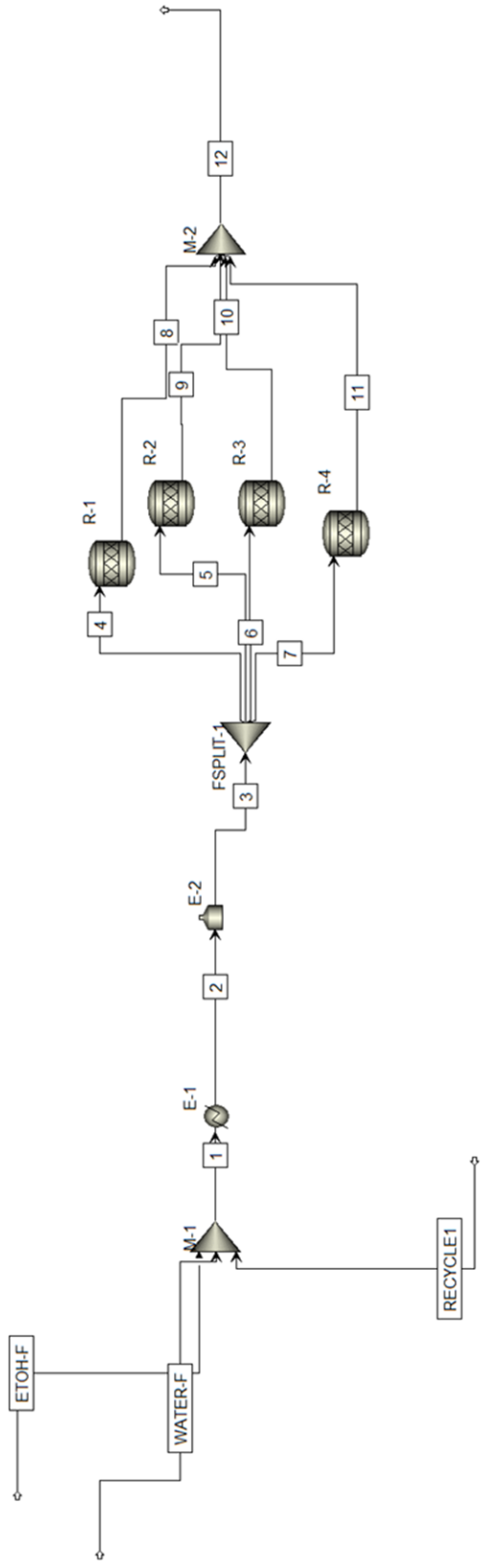
Figure 9 Process Flow Diagram for the Reactor Section in the Production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst.
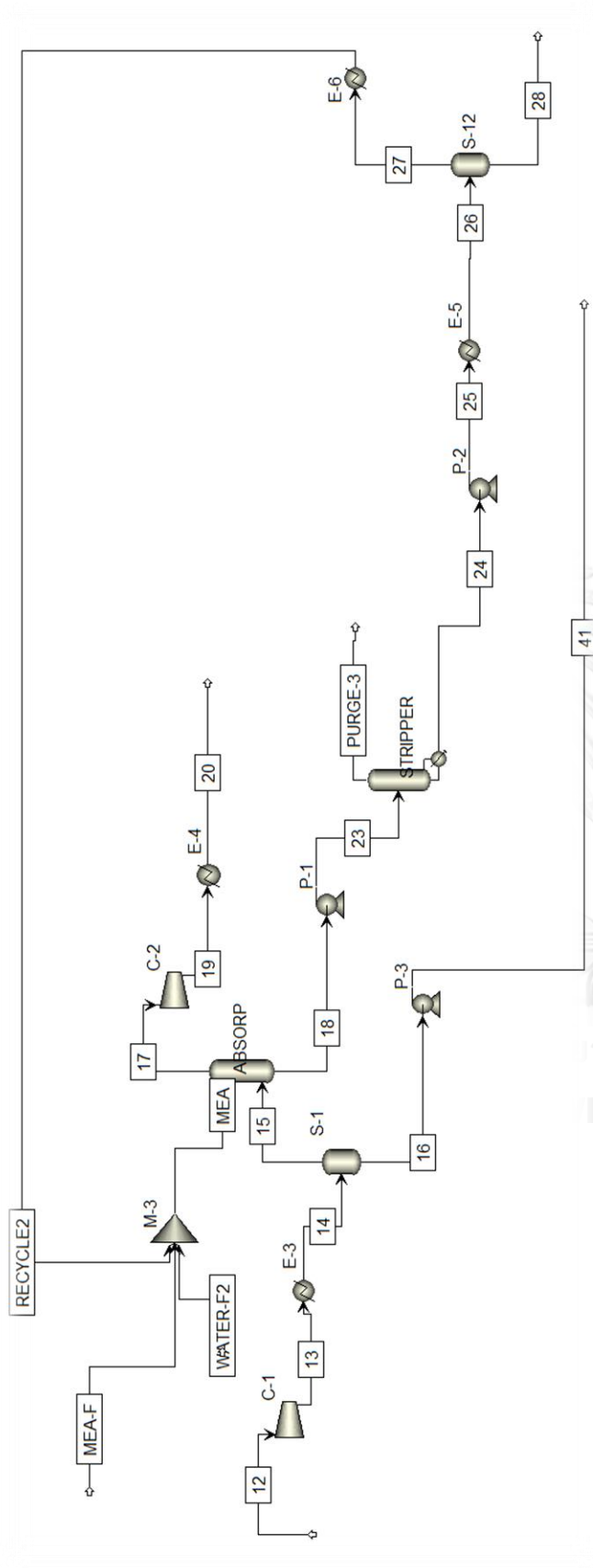
Figure 10: Process Flow Diagram for the reactive absorption and stripping section in the Production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst.

Figure 11 : Process Flow Diagram for the cryogenic distillation section in the Production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst.
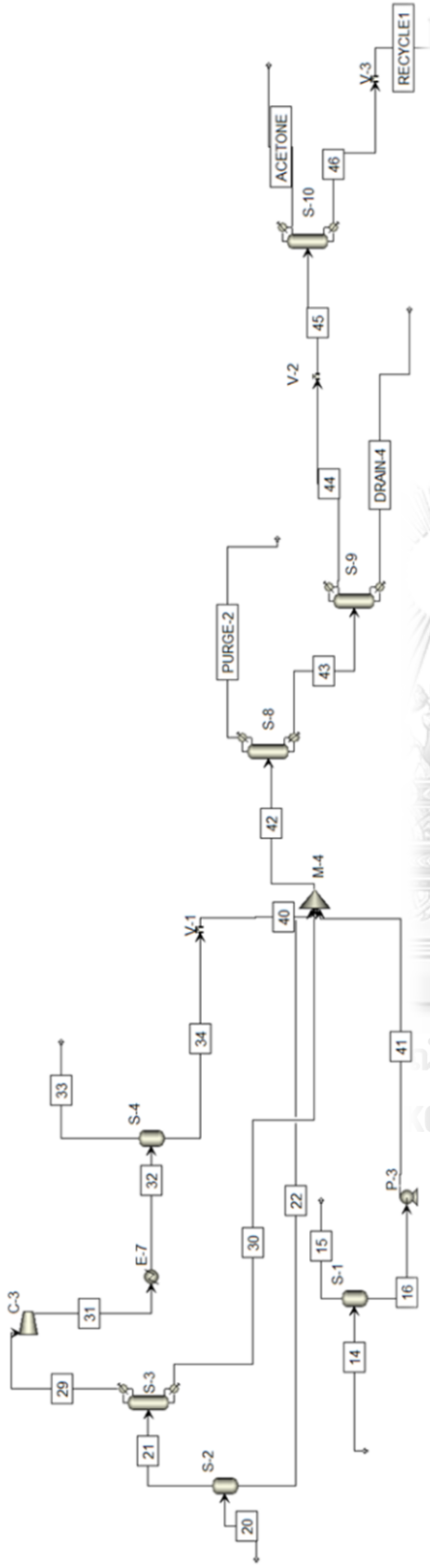
Figure 12: Process Flow Diagram for the distillation section in the Production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst.

3.5 Economic analysis

In this study, Table 10 lists the cost assumptions for raw materials, products, and catalysts used in the feasibility calculations, while Table 11 outlines the utility cost assumptions for these calculations.

Table 10 Costs of Raw Materials, Products, and Catalysts

Item	Detail	Cost	Unit	Reference
1.	Ethanol 95%	1.05	USD/kg	[5]
2.	Acetone 95%	2.91	USD/kg	[6]
3.	Ethylene 99%	12.77	USD/kg	[7]
4.	Water	0.6943	USD/m³	[37]
5.	MEA 90%	2.4592	USD/kg	[38]
6.	ZnO catalyst	4287	USD/ton	[39]
7.	CaO catalyst	67.16	USD/ton	[40]

Table 11 Costs of Utilities

Item	Utility	Unit	Case I (ZnO-CaO catalyst)	Case II (ZnO catalyst)	Reference
			Cost		
1.	Electricity	USD/kWh	0.0775	0.0775	Aspen
2.	Cooling water	USD/m³	0.0317	0.0317	[41]
3.	Medium pressure steam	USD/GJ	2.78	2.78	
4.	High pressure steam	USD/ton	-	25.77	
5.	Chilled water	USD/ton	0.185	0.185	
6.	Natural Gas	USD/GJ	3.16	3.16	
7.	Propylene refrigerant	USD/GJ	-	43.2	[42]
8.	C1/C2/C3 refrigerant	USD/GJ	-	135	[42]

In the final analysis, sizing of unit operations, including cost estimations for all equipment in the acetone and ethylene production processes, was performed for both cases using Aspen Process Economic Evaluation. This analysis yielded the Net Present Value (NPV), Internal Rate of Return (IRR), Profitability Index (PI), and Payback Period (PP)

Net present value (NPV) [43]

$$\text{NPV} = \sum_{t=0}^{N} \frac{CF_t}{(1+r)^t} \tag{3.3}$$

CF_t represents the anticipated net cash flow at time t. For this project, the projected lifespan (N) is assumed to be 20 years, and the discount rate (r) is assumed to be 10%. An NPV greater than 0 indicates that the project is financially viable and potentially worth investing in.

Internal Rate of Return (IRR) [44]

$$\text{IRR} = \sum_{t=0}^{N} \frac{CF_t}{(1+IRR)^t} = 0 \tag{3.4}$$

An IRR greater than r (discount rate) indicates that the project is financially viable and potentially worth investing in.

Profitability Index (PI) [45]

$$\text{PI} = \frac{Present\ Value\ (PV) of\ Future\ Cash\ Flows}{Initial\ Investment} \tag{3.5}$$

An PI greater than 1 indicates that the project is financially viable and potentially worth investing in.

CHAPTER 4

Results and Discussion

This chapter includes an explanation and discussion of the study's results. It covers six topics: evaluation of raw material utilization, simulation results, heat recovery systems, and economic assessment.

4.1 Evaluation of raw material utilization

In this study, mass balance calculations are utilized to evaluate the amount of feed before simulating the process using Aspen Plus® V11. These calculations consider the stoichiometric ratios of the chemical reactions from Equations (2.1) to (2.4), as well as the conversion and yield data from Table 6, with item 1 pertaining to Case I and item 2 to Case II. In table 12 and 13 presents mass flow rates to the mixer in Case I and Case II as determined by the mass balance calculations and the simulation results.

Table 12 Comparison of the mass flow rates to the mixer in Case I as determined by the mass balance calculations and the simulation results.

Stream name	Substance	Mass balance calculations	Simulation results.
		Mass flowrate (tons/year)	
ETOH-F	Ethanol	87,154.23	87,156.097
	Water	4,587.06	4,587.163
WATER-F	Water	7,860.84	10,375.594
RECYCLE	Water	142,492.95	139,857.334
	Acetone	-	3.3654E-09
	Ethylene	-	1.28654E-41
	CO_2	-	1.00691E-32
	H_2	-	5.50262E-47

Table 13 Comparison of the mass flow rates to the mixer in Case II as determined by the mass balance calculations and the simulation results.

Stream name	Substance	Mass balance calculations	Simulation results.
		Mass flowrate (tons/year)	
ETOH-F	Ethanol	85,934.07	86,822.6254
	Water	4,522.85	4,569.61186
WATER-F	Water	-	146,113.8054
RECYCLE1	Ethanol	1,220.16	333.4336
	Water	150,418.01	4256.5057
	Acetone	-	8.46082E-06

Table 12 shows discrepancies between the substances and mass flow rates in mass balance calculations compared to simulation results. This variance stems from the assumption in mass balance calculations that separation is perfect, meaning that all water in the process can be completely separated and recycled as the recycle stream (RECYCLE). However, the simulation results indicate that water is present not only in the recycle stream but also as a component in other streams. Additionally, there are trace amounts of acetone, ethylene, CO_2, and H_2 in the recycle stream, which suggests that the separation is not entirely perfect.

Table 13 shows discrepancies between the substances and mass flow rates in mass balance calculations compared to simulation results. This variance stems from the assumption in mass balance calculations that separation is perfect, meaning that all water and ethanol in the process can be completely separated and recycled as the recycle stream (RECYCLE1). However, the simulation results indicate that water and ethanol is present not only in the recycle stream but also as a component in other streams. Additionally, there are trace amounts of acetone in the recycle stream, which suggests that the separation is not entirely perfect.

4.2 Simulation results

From process flow diagram in chapter 3 in section 3.4, stream results via Aspen Plus® V11. In table 14 presents acetone production from bioethanol with ZnO-CaO catalyst (Case I) and table 15 presents acetone and ethylene production from bioethanol with ZnO catalyst (Case II).

Table 14 Simulation results of acetone production from bioethanol with ZnO-CaO catalyst (Case I).

	Units	1	2	3	4	5	6	7
From		M-1	E-1	E-2	FSPLIT-1	FSPLIT-1	FSPLIT-1	FSPLIT-1
To		E-1	E-2	FSPLIT-1	R-1	R-2	R-3	R-4
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	79.0039	239	400	400	400	400	400
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Mass Vapor Fraction		-	1	1	1	1	1	1
Mass Liquid Fraction		1	-	-	-	-	-	-
Mass Flows	kg/hr	25041.88	25041.88	25041.88	6260.47	6260.47	6260.47	6260.47
ACETONE	kg/hr	3.48E-10	3.48E-10	3.48E-10	8.71E-11	8.71E-11	8.71E-11	8.71E-11
WATER	kg/hr	16022.18	16022.18	16022.18	4005.545	4005.545	4005.545	4005.545
ETHANOL	kg/hr	9019.699	9019.699	9019.699	2254.925	2254.925	2254.925	2254.925
ETHYLENE	kg/hr	1.33E-42	1.33E-42	1.33E-42	3.33E-43	3.33E-43	3.33E-43	3.33E-43
CO2	kg/hr	1.04E-33	1.04E-33	1.04E-33	2.61E-34	2.61E-34	2.61E-34	2.61E-34
H2	kg/hr	5.69E-48	5.69E-48	5.69E-48	1.42E-48	1.42E-48	1.42E-48	1.42E-48

	Units	8	9	10	11	12	13	14
From		R-1	R-2	R-3	R-4	M-2	C-1	E-3
To		M-2	M-2	M-2	M-2	C-1	E-3	E-4
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	400	400	400	400	400	636.4515	32
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	5.06625	5.06625
Mass Vapor Fraction		1	1	1	1	1	1	0.238358
Mass Liquid Fraction		-	-	-	-	-	-	0.761642
Mass Flows	kg/hr	6260.47	6260.47	6260.47	6260.47	25041.88	25041.88	25041.88
ACETONE	kg/hr	1293.484	1293.484	1293.484	1293.484	5173.938	5173.938	5173.938
WATER	kg/hr	3683.692	3683.692	3683.692	3683.692	14734.77	14734.77	14734.77
ETHANOL	kg/hr	-	-	-	-	-	-	-
ETHYLENE	kg/hr	123.5824	123.5824	123.5824	123.5824	494.3294	494.3294	494.3294
CO2	kg/hr	980.13	980.13	980.13	980.13	3920.52	3920.52	3920.52
H2	kg/hr	179.5804	179.5804	179.5804	179.5804	718.3216	718.3216	718.3216

	Units	15	16	17	18	ACETONE	ETOH-F	PURGE-1
From		E-4	S-1	V-1	S-2	S-2		S-1
To		S-1	V-1	S-2	V-2		M-1	
Phase			Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase
Temperature	C	23	23	22.93651	109.735	44.89199	30	23
Pressure	bar	5.06625	5.06625	1.41855	1.41855	1.2159	1.01325	5.06625
Mass Vapor Fraction		0.224751	-	0.000537	-	-	-	1
Mass Liquid Fraction		0.775249	1	0.999463	1	1	1	-
Mass Flows	kg/hr	25041.88	19413.7	19413.7	14473.7	4851.009	9494.42	5628.181
ACETONE	kg/hr	5173.938	4666.069	4666.069	1.83E-11	4612.262	-	507.8689
WATER	kg/hr	14734.77	14690.95	14690.95	14473.7	216.0173	474.721	43.82168
ETHANOL	kg/hr	-	-	-	-	-	9019.699	-
ETHYLENE	kg/hr	494.3294	1.29113	1.29113	9.63E-47	0.413955	-	493.0383
CO2	kg/hr	3920.52	55.17752	55.17752	3.83E-37	22.31057	-	3865.342
H2	kg/hr	718.3216	0.212131	0.212131	1.67E-52	0.004288	-	718.1095

	Units	PURGE-2	RECYCLE1	WATER-F
From		S-2	M-1	M-1
To				M-1
Phase		Vapor Phase	Liquid Phase	Liquid Phase
Temperature	C	44.89199	100.0178	30
Pressure	bar	1.2159	1.01325	1.01325
Mass Vapor Fraction		1	-	-
Mass Liquid Fraction		-	1	-
Mass Flows	kg/hr	89.02732	14473.7	1073.76
ACETONE	kg/hr	53.85758	3.48E-10	-
WATER	kg/hr	1.217146	14473.7	1073.76
ETHANOL	kg/hr	-	-	-
ETHYLENE	kg/hr	0.877189	1.33E-42	-
CO2	kg/hr	32.86755	1.04E-33	-
H2	kg/hr	0.207845	5.69E-48	-

Table 15 Simulation results of acetone and ethylene production from bioethanol with ZnO catalyst (Case II).

Reactor Section

	Units	1	2	3	4	5	6	7
From		M-1	E-1	E-2	FSPLIT-1	FSPLIT-1	FSPLIT-1	FSPLIT-1
To		E-1	E-2	FSPLIT-1	R-1	R-2	R-3	R-4
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	34.43168	239	400	400	400	400	400
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Mass Vapor Fraction		-	1	1	1	1	1	1
Mass Liquid Fraction		1	-	-	-	-	-	-
Mass Flows	kg/hr	25054.28	25054.28	25054.28	6263.569	6263.569	6263.569	6263.569
ETHANOL	kg/hr	9019.695	9019.695	9019.695	2254.924	2254.924	2254.924	2254.924
WATER	kg/hr	16034.58	16034.58	16034.58	4008.645	4008.645	4008.645	4008.645
ACETONE	kg/hr	8.76E-07	8.76E-07	8.76E-07	2.19E-07	2.19E-07	2.19E-07	2.19E-07
CO2	kg/hr	-	-	-	-	-	-	-
H2	kg/hr	-	-	-	-	-	-	-
ACETA-01	kg/hr	-	-	-	-	-	-	-
ETHYLENE	kg/hr	-	-	-	-	-	-	-
MEA	kg/hr	-	-	-	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-	-	-

	Units	8	9	10	11	12	ETOH-F	RECYCLE1	WATER-F
From		R-1	R-2	R-3	R-4	M-2	M-1	M-1	M-1
To		M-2	M-2	M-2	M-2	C-1			
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	400	400	400	400	400	30	85.61314751	30
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Mass Vapor Fraction		1	1	1	1	1	-	-	-
Mass Liquid Fraction		-	-	-	-	-	1	1	1
Mass Flows	kg/hr	6263.569	6263.569	6263.569	6263.569	25054.28	9458.093	475.0083145	15121.17437
ETHANOL	kg/hr	31.56893	31.56893	31.56893	31.56893	126.2757	8985.188	34.50671779	-
WATER	kg/hr	4273.825	4273.825	4273.825	4273.825	17095.3	472.9046	440.515959	15121.17437
ACETONE	kg/hr	574.6195	574.6195	574.6195	574.6195	2298.478	-	8.76E-07	-
CO2	kg/hr	435.4145	435.4145	435.4145	435.4145	1741.658	-	-	-
H2	kg/hr	87.56021	87.56021	87.56021	87.56021	350.2408	-	-	-
ACETA-01	kg/hr	170.0853	170.0853	170.0853	170.0853	680.341	-	-	-
ETHYLENE	kg/hr	690.4955	690.4955	690.4955	690.4955	2761.982	-	-	-
MEA	kg/hr	-	-	-	-	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-	-	-	-

Units		13	14	15	16	17	18	23
From		C-1	E-3	S-1	S-1	ABSORP	ABSORP	P-1
To		E-3	S-1	ABSORP	P-3	C-2	P-1	STRIPPER
Phase		Vapor Phase		Vapor Phase	Liquid Phase	Vapor Phase	Liquid Phase	Liquid Phase
Temperature	C	412.47314	75	75	75	101.11951	100.8626	100.85908
Pressure	bar	1.114575	1.114575	1.114575	1.114575	1.01325	1.01325	1.114575
Mass Vapor Fraction		1	0.4359284	1	-	1	-	-
Mass Liquid Fraction		-	0.5640716	-	1	-	1	1
Mass Flows	kg/hr	25054.276	25054.276	10921.871	14132.405	9679.6792	10054.218	10054.218
ETHANOL	kg/hr	126.27573	126.27573	93.749349	32.526382	74.395605	19.582567	19.582567
WATER	kg/hr	17095.3	17095.3	3393.6785	13701.621	3959.9064	2596.2853	2596.2853
ACETONE	kg/hr	2298.4781	2298.4781	2068.4404	230.03768	1716.132	359.47507	359.47507
CO2	kg/hr	1741.6579	1741.6579	1692.3159	49.341991	90.677481	29.16295	29.16295
H2	kg/hr	350.24085	350.24085	350.24084	6.53E-06	350.24083	8.77E-06	8.77E-06
ACETA-01	kg/hr	680.34103	680.34103	657.3788	22.962222	601.37646	56.362875	56.362875
ETHYLENE	kg/hr	2761.9821	2761.9821	2666.0672	95.914922	2604.8977	61.241921	61.241921
MEA	kg/hr	-	-	-	-	282.05279	1135.4271	1135.4271
CO3-2	kg/hr	-	-	-	-	-	0.0108004	0.0108004
H3O+	kg/hr	-	-	-	-	-	5.37E-05	5.37E-05
HCO3-	kg/hr	-	-	-	-	-	199.68949	199.68949
MEAH+	kg/hr	-	-	-	-	-	2218.5694	2218.5694
MEACOO-	kg/hr	-	-	-	-	-	3378.4103	3378.4103
OH-	kg/hr	-	-	-	-	-	0.0005098	0.0005098

Reactive absorption and stripping section

	Units	24	25	26	27	28	41	MEA-F
From		STRIPPER	P-2	E-5	S-12	S-12	P-3	M-3
To		P-2	E-5	S-12	E-6		M-4	
Phase		Liquid Phase	Liquid Phase		Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	193.19505	193.19956	305.57457	305.57457	305.57457	75.119565	35
Pressure	bar	1.01325	1.114575	1.114575	1.114575	1.114575	6.0795	1.114575
Mass Vapor Fraction		-	-	0.1814487	1	-	-	-
Mass Liquid Fraction		1	1	0.8185513	-	1	1	1
Mass Flows	kg/hr	7309.2173	7309.2173	7309.2173	1326.2477	5982.9695	14132.405	5327.4667
ETHANOL	kg/hr	0.2384885	0.2384885	0.2384885	0.2287601	0.0097284	32.526382	-
WATER	kg/hr	623.3369	623.3369	623.3369	531.08418	92.252724	13701.621	532.74667
ACETONE	kg/hr	7.5850205	7.5850205	7.5850205	7.1709183	0.4141021	230.03768	-
CO2	kg/hr	0.0238974	0.0238974	0.0238974	0.0238103	8.71E-05	49.341991	-
H2	kg/hr	2.29E-19	2.29E-19	2.29E-19	-	-	6.53E-06	-
ACETA-01	kg/hr	0.374238	0.374238	0.374238	0.3609305	0.0133075	22.962222	-
ETHYLENE	kg/hr	0.072934	0.072934	0.072934	0.0725228	0.0004112	95.914922	-
MEA	kg/hr	880.90651	880.90651	880.90651	787.30662	93.599896	-	4794.7201
CO3-2	kg/hr	0.0108004	0.0108004	0.0108004	-	0.0108004	-	-
H3O+	kg/hr	5.37E-05	5.37E-05	5.37E-05	-	5.37E-05	-	-
HCO3-	kg/hr	199.68945	199.68945	199.68945	-	199.68945	-	-
MEAH+	kg/hr	2218.5689	2218.5689	2218.5689	-	2218.5689	-	-
MEACOO-	kg/hr	3378.4096	3378.4096	3378.4096	-	3378.4096	-	-
OH-	kg/hr	0.0005098	0.0005098	0.0005098	-	0.0005098	-	-

	Units	PURGE-3	RECYCLE2	WATER-F2
From		STRIPPER	M-3	M-3
To				
Phase		Vapor Phase	Liquid Phase	Liquid Phase
Temperature	C	136.74553	100.3405737	35
Pressure	bar	1.01325	1.114575	1.114575
Mass Vapor Fraction		1	-	-
Mass Liquid Fraction		-	1	1
Mass Flows	kg/hr	2745	1327.345542	2157.2142
ETHANOL	kg/hr	19.344082	0.228823269	0
WATER	kg/hr	1972.9486	531.5138462	2157.2142
ACETONE	kg/hr	351.89012	7.166593929	-
CO2	kg/hr	29.139058	0.023795275	-
H2	kg/hr	8.77E-06	-	-
ACETA-01	kg/hr	55.988647	0.360527379	-
ETHYLENE	kg/hr	61.168999	0.072473325	-
MEA	kg/hr	254.52048	787.9794823	-
CO3-2	kg/hr	4.30E-28	-	-
'H3O+	kg/hr	2.14E-30	-	-
HCO3-	kg/hr	7.96E-24	-	-
MEAH+	kg/hr	8.84E-23	-	-
MEACOO-	kg/hr	1.35E-22	-	-
OH-	kg/hr	2.03E-29	-	-

Cryogenic distillation section

	Units	19	20	21	22	29	30	31
From		C-2	E-4	S-2	S-2	S-3	S-3	C-3
To		E-4	S-2	S-3	M-4	C-3	M-4	E-7
Phase		Vapor Phase		Vapor Phase	Liquid Phase	Vapor Phase	Liquid Phase	Vapor Phase
Temperature	C	259.14466	117.01901	117.01901	117.01901	-29.63347	106.65219	35.382729
Pressure	bar	6.0795	6.0795	6.0795	6.0795	5.87685	6.0795	15.19875
Mass Vapor Fraction		1	0.7719429	1	-	1	-	1
Mass Liquid Fraction		-	0.2280571	-	1	-	1	-
Mass Flows	kg/hr	9679.6792	9679.6792	7472.1599	2207.5193	3479.9826	3992.1708	3479.9826
ETHANOL	kg/hr	74.395605	74.395605	68.777044	5.6185613	0.2042664	68.572558	0.2042664
WATER	kg/hr	3959.9064	3959.9064	2172.1122	1787.7942	1.345938	2170.7593	1.345938
ACETONE	kg/hr	1716.132	1716.132	1649.1733	66.958703	165.56904	1483.5998	165.56904
CO2	kg/hr	90.677481	90.677481	88.763854	1.913627	88.233537	0.5304719	88.233537
H2	kg/hr	350.24083	350.24083	350.24081	1.60E-05	350.24144	1.39E-14	350.24144
ACETA-01	kg/hr	601.37646	601.37646	593.54646	7.8300005	353.79201	239.75431	353.79201
ETHYLENE	kg/hr	2604.8977	2604.8977	2536.0632	68.834493	2520.5963	15.471362	2520.5963
MEA	kg/hr	282.05279	282.05279	13.483062	268.56973	6.91E-06	13.483012	6.91E-06
CO3-2	kg/hr	-	-	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-	-	-

	Units	32	33	34	35	36	37	38
From		E-7	S-4	S-4	C-4	S-5	V-4	S-6
To		S-4	C-4	V-1	S-5	V-4	S-6	C-5
Phase			Vapor Phase	Liquid Phase	Vapor Phase	Liquid Phase	Vapor Phase	Vapor Phase
Temperature	C	6.2661526	6.2661526	6.2661526	22.110222	-26.89549	-34.7354	-33.06328
Pressure	bar	15.19875	15.19875	15.19875	18.947775	18.947775	15.19875	14.1855
Mass Vapor Fraction		0.9273096	1	-	1	-	0.069558	1
Mass Liquid Fraction		0.0726904	-	1	-	1	0.930442	-
Mass Flows	kg/hr	3479.9826	3227.0211	252.96141	3227.0211	2827.0196	2827.0196	2449.9998
ETHANOL	kg/hr	0.2042664	0.0110358	0.1932306	0.0110358	0.0110358	0.0110358	3.48E-07
WATER	kg/hr	1.345938	0.1118645	1.2340735	0.1118645	0.1118645	0.1118645	2.97E-06
ACETONE	kg/hr	165.56904	55.30589	110.26315	55.30589	55.30589	55.30589	0.083391
CO2	kg/hr	88.233537	87.327498	0.9060398	87.327498	86.970032	86.970032	83.749676
H2	kg/hr	350.24144	350.24144	1.57E-07	350.24144	0.0014575	0.0014575	0.0014575
ACETA-01	kg/hr	353.79201	240.57066	113.22135	240.57066	240.57066	240.57066	4.4408107
ETHYLENE	kg/hr	2520.5963	2493.4528	27.143559	2493.4528	2444.0487	2444.0487	2361.7245
MEA	kg/hr	6.91E-06	2.38E-09	6.90E-06	2.38E-09	2.38E-09	2.38E-09	1.58E-16
CO3-2	kg/hr	-	-	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-	-	-

	Units	39	40	41	DRAIN-1	DRAIN-2	ETHYLENE	PURGE-1
From		C-5	V-1	P-3	S-6	S-7	S-7	S-5
To		S-7	M-4	M-4				
Phase		Vapor Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase	Vapor Phase
Temperature	C	-31.77755	5.9551681	75.119565	47.002693	-33.60269	-41.19702	-132.601
Pressure	bar	14.489475	6.0795	6.0795	15.19875	14.489475	13.98285	18.339825
Mass Vapor Fraction		1	4.41E-08	-	-	-	1	1
Mass Liquid Fraction		-	-	1	1	1	-	-
Mass Flows	kg/hr	2449.9998	252.96141	14132.405	377.01756	142.99985	2307	400.00154
ETHANOL	kg/hr	3.48E-07	0.1932306	32.526382	0.0110353	3.48E-07	1.79E-54	9.88E-17
WATER	kg/hr	2.97E-06	1.2340735	13701.621	0.1118594	2.97E-06	2.08E-59	4.23E-14
ACETONE	kg/hr	0.083391	110.26315	230.03768	55.221405	0.0833911	4.94E-36	4.08E-08
CO2	kg/hr	83.749676	0.9060398	49.341991	3.2204714	81.656159	2.0935957	0.357466
H2	kg/hr	0.0014575	1.57E-07	6.53E-06	5.91E-20	1.38E-142	0.0014575	350.23998
ACETA-01	kg/hr	4.4408107	113.22135	22.962222	236.12518	4.440815	2.99E-26	5.03E-06
ETHYLENE	kg/hr	2361.7245	27.143559	95.914922	82.327607	56.819484	2304.905	49.404085
MEA	kg/hr	1.58E-16	6.90E-06	-	2.38E-09	-	-	8.68E-27
CO3-2	kg/hr	-	-	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-	-	-

Distillation section

	Units	14	15	16	17	20	21	22
From		E-3	S-1	S-1	ABSORP	E-4	S-2	S-2
To		S-1	ABSORP	P-3	C-2	S-2	S-3	M-4
Phase			Vapor Phase	Liquid Phase	Vapor Phase	S-2	Vapor Phase	Liquid Phase
Temperature	C	75	75	75	101.11951	117.01901	117.01901	117.01901
Pressure	bar	1.114575	1.114575	1.114575	1.01325	6.0795	6.0795	6.0795
Mass Vapor Fraction		0.4359284	1	-	1	0.7719429	1	-
Mass Liquid Fraction		0.5640716	-	1	-	0.2280571	-	1
Mass Flows	kg/hr	25054.276	10921.871	14132.405	9679.6792	9679.6792	7472.1599	2207.5193
ETHANOL	kg/hr	126.27573	93.749349	32.526382	74.395605	74.395605	68.777044	5.6185613
WATER	kg/hr	17095.3	3393.6785	13701.621	3959.9064	3959.9064	2172.1122	1787.7942
ACETONE	kg/hr	2298.4781	2068.4404	230.03768	1716.132	1716.132	1649.1733	66.958703
CO2	kg/hr	1741.6579	1692.3159	49.341991	90.677481	90.677481	88.763854	1.913627
H2	kg/hr	350.24085	350.24084	6.53E-06	350.24083	350.24083	350.24081	1.60E-05
ACETA-01	kg/hr	680.34103	657.3788	22.962222	601.37646	601.37646	593.54646	7.8300005
ETHYLENE	kg/hr	2761.9821	2666.0672	95.914922	2604.8977	2604.8977	2536.0632	68.834493
MEA	kg/hr	-	-	-	-	282.05279	13.483062	268.56973
CO3-2	kg/hr	-	-	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-	-	-

	Units	23	29	30	31	32	33	34
From		P-1	S-3	S-3	C-3	E-7	S-4	S-4
To		STRIPPER	C-3	M-4	E-7	S-4	C-4	V-1
Phase		Liquid Phase	Vapor Phase	Liquid Phase	Vapor Phase		Vapor Phase	Liquid Phase
Temperature	C	100.85908	-29.63347	106.65219	35.382729	6.2661526	6.2661526	6.2661526
Pressure	bar	1.114575	5.87685	6.0795	15.19875	15.19875	15.19875	15.19875
Mass Vapor Fraction		-	1	-	1	0.9273096	1	-
Mass Liquid Fraction		1	-	1	-	0.0726904	-	1
Mass Flows	kg/hr	10054.218	3479.9826	3992.1708	3479.9826	3479.9826	3227.0211	252.96141
ETHANOL	kg/hr	19.582567	0.2042664	68.572558	0.2042664	0.2042664	0.0110358	0.1932306
WATER	kg/hr	2596.2853	1.345938	2170.7593	1.345938	1.345938	0.1118645	1.2340735
ACETONE	kg/hr	359.47507	165.56904	1483.5998	165.56904	165.56904	55.30589	110.26315
CO2	kg/hr	29.16295	88.233537	0.5304719	88.233537	88.233537	87.327498	0.9060398
H2	kg/hr	8.77E-06	350.24144	1.39E-14	350.24144	350.24144	350.24144	1.57E-07
ACETA-01	kg/hr	56.362875	353.79201	239.75431	353.79201	353.79201	240.57066	113.22135
ETHYLENE	kg/hr	61.241921	2520.5963	15.471362	2520.5963	2520.5963	2493.4528	27.143559
MEA	kg/hr	1135.4271	6.91E-06	13.483012	6.91E-06	6.91E-06	2.38E-09	6.90E-06
CO3-2	kg/hr	0.0108004	-	-	-	-	-	-
H3O+	kg/hr	5.37E-05	-	-	-	-	-	-
HCO3-	kg/hr	199.68949	-	-	-	-	-	-
MEAH+	kg/hr	2218.5694	-	-	-	-	-	-
MEACOO-	kg/hr	3378.4103	-	-	-	-	-	-
OH-	kg/hr	0.0005098	-	-	-	-	-	-

	Units	40	41	42	43	44	45	46
From		V-1	P-3	M-4	S-8	S-9	V-2	S-10
To		M-4	M-4	S-8	S-9	V-2	S-10	V-3
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase		Liquid Phase
Temperature	C	5.9551681	75.119565	85.106066	142.66069	107.44622	64.047347	98.225923
Pressure	bar	6.0795	6.0795	6.0795	6.0795	5.06625	1.2159	1.2159
Mass Vapor Fraction		4.41E-08	-	-	-	-	0.2044157	-
Mass Liquid Fraction		1	1	1	1	1	0.7955843	1
Mass Flows	kg/hr	252.96141	14132.405	20585.056	19924.736	2455.0084	2455.0084	475.00843
ETHANOL	kg/hr	0.1932306	32.526382	106.91073	106.89364	106.89419	106.89419	33.935658
WATER	kg/hr	1.2340735	13701.621	17661.409	17656.822	469.13701	469.13701	441.07277
ACETONE	kg/hr	110.26315	230.03768	1890.8593	1878.6929	1878.7025	1878.7025	8.44E-07
CO2	kg/hr	0.9060398	49.341991	52.69213	0.0021533	0.0021533	0.0021533	4.03E-30
H2	kg/hr	1.57E-07	6.53E-06	2.27E-05	1.59E-102	-	-	-
ACETA-01	kg/hr	113.22135	22.962222	383.76788	0.004397	0.004397	0.004397	1.29E-16
ETHYLENE	kg/hr	27.143559	95.914922	207.36434	0.2681805	0.2681819	0.2681819	1.80E-26
MEA	kg/hr	6.90E-06	-	282.05275	282.05275	5.65E-27	5.65E-27	-
CO3-2	kg/hr	-	-	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-	-	-

Units	ACETONE	DRAIN-4	PURGE-2	RECYCLE1
From	S-10	S-9	S-8	
To				M-1
Phase	Liquid Phase	Liquid Phase	Vapor Phase	Liquid Phase
Temperature C	56.366859	159.61289	51.291841	85.61314751
Pressure bar	1.01325	6.0795	5.06625	1.01325
Mass Vapor Fraction	-	-	1	-
Mass Liquid Fraction	1	1	-	1
Mass Flows kg/hr	1980.0002	17469.735	660.32	475.0083145
ETHANOL kg/hr	72.958534	3.51E-08	0.0170895	34.50671779
WATER kg/hr	28.064155	17187.682	4.5868602	440.5015959
ACETONE kg/hr	1878.7027	1.51E-08	12.16642	8.76E-07
CO2 kg/hr	0.0021533	1.88E-13	52.689976	-
H2 kg/hr	-	0	2.27E-05	-
ACETA-01 kg/hr	0.004397	1.79E-19	383.76348	-
ETHYLENE kg/hr	0.2681819	2.48E-10	207.09615	-
MEA kg/hr	-	282.05265	1.50E-06	-
CO3-2 kg/hr	-	-	-	-
H3O+ kg/hr	-	-	-	-
HCO3- kg/hr	-	-	-	-
MEAH+ kg/hr	-	-	-	-
MEACOO- kg/hr	-	-	-	-
OH- kg/hr	-	-	-	-

4.3 Performance analysis

The complexity of the process in the first case is lower than that of the second case. In the first case, the only product is acetone, which can be purified through the distillation process. In contrast, the second case involves producing ethylene and acetone. To separate ethylene from CO_2 and H_2, absorption-stripping is employed, using an amine-based solution to isolate CO_2. Cryogenic distillation, a low-temperature distillation technique, is then used to separate ethylene and H_2. Meanwhile, acetone is purified using the distillation process. Consequently, producing acetone and ethylene from bioethanol is more complex than producing acetone alone from bioethanol.

4.4 Heat recovery system

In Case I with heat recovery, as shown in Figure 13, the process of synthesizing acetone from bioethanol using a ZnO-CaO catalyst. A fresh ethanol feed (ETOH-F) with a 95% concentration, water (WATER-F), and a recycle stream (RECYCLE) are merged in mixer M-1 to create a consistent stream. Annually, this stream consists of 87,154.23 tons of ethanol and 154,940.84 tons of water, and it leads to the production of 50,000 tons of acetone. Prior to entry into the reactors R-1, R-2, and R-3, the mixture is progressively preheated in heat exchangers E-1 to E-4 to a temperature of 400°C. The resulting mixture, now containing acetone, water, ethylene, CO_2, and H_2, is unified again in mixer M-2. This mixture is then passed through heat exchanger E-1, which facilitates a heat exchange: cooling the product stream while concurrently warming the feed stream. After leaving heat exchanger E-1, the product stream is still in vapor form. To initiate a phase change to both liquid and vapor (binary phase), the vapor is compressed in compressor C-1 to increase the pressure. It is then channeled through heat exchangers E-2 and E-3 for additional heat exchange with the feed stream, resulting in further cooling. The cooling continues in heat exchangers E-5 and E-6 via heat exchange with cooling water and chilled water, respectively. Once it exits heat exchanger E-6, the product stream is conveyed to phase separator S-1, which segregates the vapor and liquid phases. The vapor phase is removed (PURGE-1), while the liquid phase, containing acetone, water,

and trace amounts of ethylene, CO_2, and H_2, is collected. This liquid is then sent through valve V-1 to decrease its pressure and subsequently fed into the distillation column S-2. From the top of the column, minor quantities of ethylene, CO_2, and H_2 are eliminated (PURGE-2), and the acetone is refined to a desired purity of 95%. Water is drawn from the bottom of the distillation column and is pressure-reduced via a valve before being looped back into the process as part of the recycle stream.

In case II with heat recovery, as shown in Figure 14 to 17, the process of producing acetone and ethylene from bioethanol using a ZnO catalyst. The ethanol feed (ETOH-F) at a 95% concentration is mixed with water (WATER-F) and a recycle stream (RECYCLE1) in mixer M-1, creating a uniform stream. This approach is consistent with the process depicted in Figure 6 (Case I), which uses a ZnO-CaO catalyst, allowing for direct comparisons of feed amounts for investment feasibility studies. Before entering reactors R-1, R-2, R-3 and R-4 f , the mixture is sequentially preheated in heat exchangers E-1 through E-4 until it reaches 400℃. The post-reaction output—including ethanol, water, acetone, acetaldehyde, ethylene, CO_2, and H_2—is consolidated in mixer M-2. This product stream is then cooled in heat exchanger E-5, simultaneously preheating the stripping stream, but it remains in vapor form. To convert the vapor to a binary liquid-vapor phase, it is compressed in compressor C-1, which increases the pressure. The pressurized vapor then cools by passing through heat exchangers E-1 and E-3, which facilitates a heat exchange—cooling the product stream while concurrently warming the feed stream. The cooling continues in heat exchangers E-6 and E-7, through heat exchange with cooling water and chilled water, respectively, before entering phase separator S-1. The heavier bottom stream from S-1 is pressurized by pump P-3 before moving on to mixer M-4. The lighter top stream (vapor phase) from S-1 is directed into the reactive absorption column (ABSORP). In mixer M-3, a 90% monoethanolamine (MEA) solution (MEA-F), additional water (WATER-F2), and another recycle stream (RECYCLE2) are combined and introduced at the top of ABSORP in a liquid phase. The vapor phase from S-1 enters the bottom of ABSORP, where the CO_2 reacts with MEA, separating from the vapor phase. After absorption, the CO_2-depleted bottom stream is pressurized by

pump P-1 and sent to the stripping column (STRIPPER) for MEA regeneration. The stream exiting STRIPPER is further pressurized by pump P-2 and rerouted through heat exchanger E-5, then proceeds to phase separator S-12, where the liquid phase is drained from the bottom, and the vapor phase is cooled in heat exchangers E-9 and E-10 with cooling water before passing through mixer M-3 as RECYCLE2, which contains water and MEA. At the top of ABSORP, trace amounts of CO_2 are compressed by C-2 and cooled in E-2. The output goes to phase separator S-2, where the liquid phase joins the flow in mixer M-4, and the vapor phase enters distillation column S-3. In S-3, the heavier bottom stream merges with the contents from M-4, while the lighter top stream is compressed by C-3, cooled in E-8 with chilled water, and then directed to phase separator S-4. The liquid phase from S-4 is depressurized through valve V-1 and routed to mixer M-4. Concurrently, the lighter top output is pressurized by C-4 and conveyed to cryogenic distillation columns S-5 to S-7, where ethylene is purified to 99% purity. The stream from mixer M-4 enters distillation columns S-8 to S-10 to concentrate the acetone to 95%. Finally, the heavy stream from the bottom of S-10 is depressurized via valve V-3 and processed through phase separator S-11. The vapor phase from S-11 is purged, and the liquid phase is recycled back to mixer M-1.
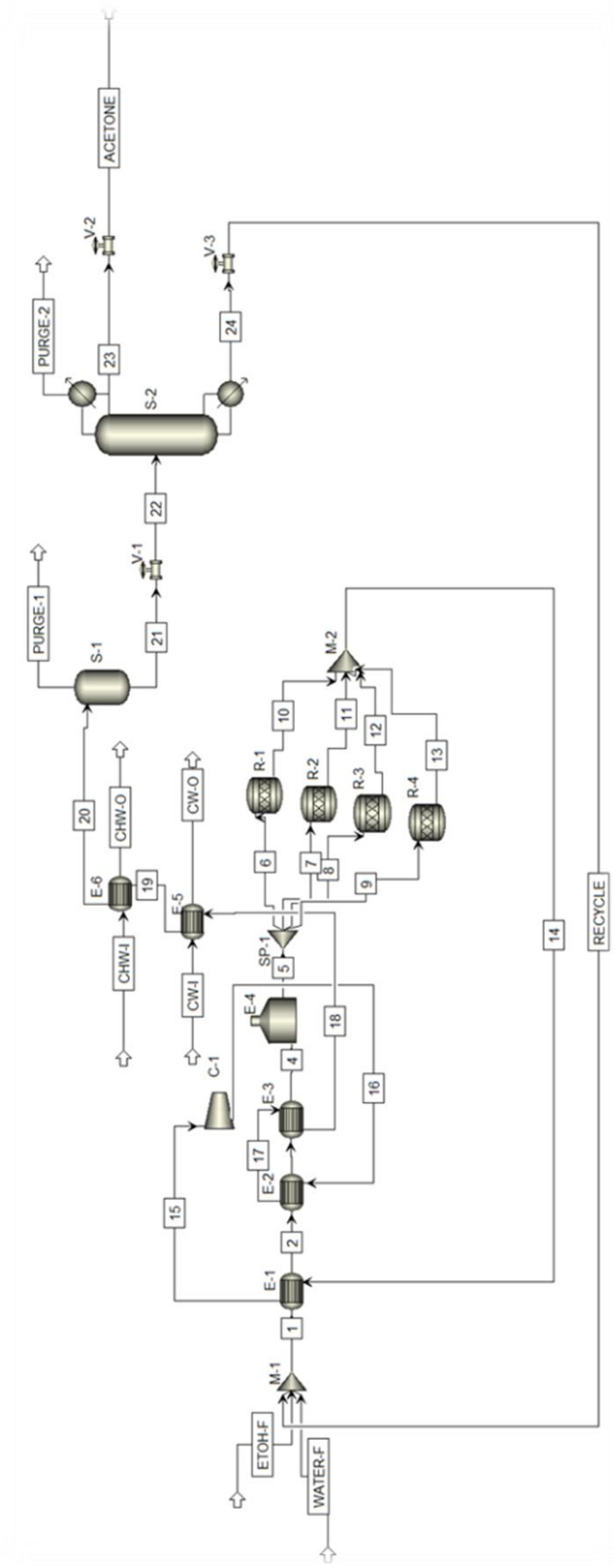
Figure 13 : Process Flow Diagram of Acetone Production from Bioethanol Using a ZnO-CaO Catalyst with Heat Exchanger Recovery.

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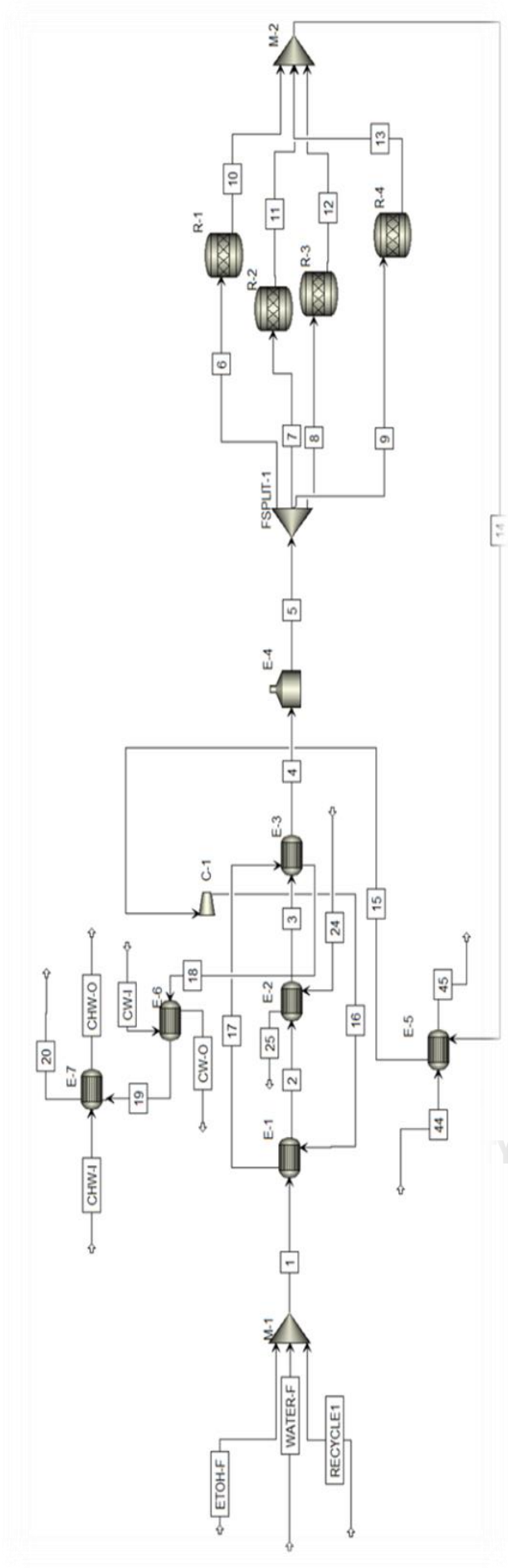
Figure 14: Process Flow Diagram for Reactor Section in the production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst with Heat Exchanger Recovery.

Figure 15: Process Flow Diagram for the reactive absorption and stripping section in the production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst with Heat Exchanger Recovery.

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Figure 16: Process Flow Diagram for the cryogenic distillation section in the production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst with Heat Exchanger Recovery.

Figure 17: Process Flow Diagram for the distillation section in the production of Acetone and Ethylene from Bioethanol Using a ZnO Catalyst with Heat Exchanger Recovery.

Table 16 presents a comparison between Case I and II, highlighting the differences in scenarios that include a heat recovery system and those that do not.

Case No.	Utility	Utility Consumption (GJ/hr)		Cost of utility consumption (USD/hr)	
		With heat recovery system	Without heat recovery system	With heat recovery system	Without heat recovery system
Case I	Cooling water	10.64	72.74	4.02	27.50
	Chilled water	4.66	1.15	3.04	0.75
	Medium pressure steam	-	52.59	-	146.20
	Natural Gas	9.03	8.57	28.53	27.07
Summary		24.33	135.05	35.59	201.52
Case II	Cooling water	8.33	60.01	3.15	22.68
	Chilled water	4.80	0.42	3.12	0.27
	High pressure steam	-	62.02	-	351.05
	Natural Gas	24.00	8.59	75.71	27.14
Summary		37.13	131.04	82.00	401.14

Table 16 indicates that the process incorporating a heat recovery system is more efficient than the process without one. This efficiency stems from the fact that the heat recovery system facilitates heat transfer for both heating and cooling with other streams in the process, reducing the reliance on external utilities for these functions.

4.5 Economic assessment

In this study, Aspen Process Economic Analyzer is used for the economic analysis. The assumption for Case I is the production of 50,000 tons/year of 95%

acetone, with a feed stream to the reactor totaling 242,095.07 tons/year. This stream has a composition of 36 wt% ethanol and 64 wt% water. In comparison, Case II maintains the same feed stream rate of 242,095.07 tons/year with an identical composition of 36 wt% ethanol and 64 wt% water. However, the product in this case includes both 95% acetone and 99% ethylene.

The economic assessment, including the costs of raw materials and catalysts, as well as the product selling price, is presented in Table 10. The annual cost estimation is provided in Table 17.

Table 17 Annual cost estimation

Detail	Case I		Case II	
	With HR	Without HR	With HR	Without HR
	Annual Cost (USD/year)			
Capital Cost	1,402,547.54	893,704.54	2,585,513.30	96,013.25
Total Raw Materials Cost	93,865,378.55	93,865,378.55	216,568,148.90	216,568,148.90
Total Utilities Cost	6,910,833.91	38,700,669.88	34,176,321.36	167,122,211.45
Total Operating Labor Cost	834,519.00	511,492.00	1,255,480.00	1,255,480.00
Total Maintenance Cost	194,036.00	81,141.20	260,396.00	258,071.00
Total Product Sale	136,491,000.00	136,491,000.00	147,289,000.00	147,289,000.00
Summary	33,283,685.00	2,868,964.63	-107,556,859.56	-238,010,924.60

Table 17 shows that the summary value is positive which mean the value of total cost is less than the value of total product sale in Case I both with heat integration and without heat integration but in without heat integration the summary is less than heat integration due to the higher cost of total utilities cost. In Case II, both with heat integration and without heat integration, the summary value is negative. This indicates that Case II is less attractive for investment due to the complexity of its processes. These include CO_2 separation using MEA solution, reactive absorption cause to the higher cost of raw material, a stripping column to recovery MEA solution, and ethylene purification through cryogenic distillation, along with higher utility costs for the condenser.

To evaluate the economic feasibility, key economic indicators such as Net Present Value (NPV), Internal Rate of Return (IRR), Profitability Index (PI), and Payback Period were analyzed, assuming a 10% discount rate, 20 years plant life as shown in Table 18.

Table 18 key economic indicators

Item	Detail	Case I		Case II	
		With HR	Without HR	With HR	Without HR
1.	NPV	171,634,839 USD	106,224,738 USD	(1,073,071,360) USD	(2,293,171,391) USD
2.	IRR	34%	23%	N/A	N/A
3.	PI	3.17	1.71	(9.25)	(21.93)
4.	Payback Period	5 years 8 months	8 years 10 months	More than 20 years	More than 20 years

Table 18 shows that Case I is economically feasible: it has a positive Net Present Value (NPV), an Internal Rate of Return (IRR) exceeding the assumed 10% discount rate, a Profitability Index (PI) greater than 1, and a payback period of 5 years and 8 months. In contrast, Case II is deemed a less attractive investment due to its payback period exceeding 20 years.

CHAPTER 5

Conclusion and Recommendation

5.1 Conclusion

The increasing trend of electric vehicles (EVs) directly affects the bioethanol market, as it leads to a decrease in gasohol demand. This decline in bioethanol usage subsequently impacts domestic agriculture. In this study, we explore the shift in the bio-based or organic chemical industry towards renewable raw materials, aligning with global warming mitigation efforts. We use Aspen Plus® V11 for process simulation, focusing on acetone and ethylene production. Additionally, the Aspen Process Economic Analyzer is employed for economic analysis.

This study examines two cases, each producing different products: acetone and ethylene. Both cases use the same amount of raw materials fed into the reactor and operate under identical conditions (400°C and 1 atm). However, they differ in the catalysts used: Case I employs a ZnO-CaO catalyst, while Case II uses a ZnO catalyst. This difference in catalysts directly affects the products obtained; Case I produces only acetone, whereas Case II yields both acetone and ethylene.

The first result involves evaluating raw material utilization by comparing mass balance calculations with simulation results for both the fresh feed stream and the recycle stream in each case. In Case I, the amount of ethanol in the feed stream is nearly identical in both calculations and simulations, as the ethanol conversion rate is 100%. However, the amount of water in the feed stream in the simulation results is higher than that in the mass balance calculations. This discrepancy arises because the separation process in the mass balance calculations is assumed to be ideal, meaning it achieves perfect separation. Consequently, the only component in the recycle stream in the mass balance calculations is water, and its quantity is higher than in the simulation results. Due to the assumption of perfect separation in the mass balance calculations, the quantities of both fresh feed (ethanol and water) and the recycle stream in Case II are lower than those in the simulation results.

The second result focuses on the simulation outcomes and performance analysis. Case II's process is more complex than Case I, as the reactor output includes acetone, ethylene, water, CO_2, and H_2. However, ethylene, CO_2, and H_2 are present only in trace amounts compared to acetone. In this case, phase separation is employed to remove all traces of ethylene, CO_2, and H_2, and a single distillation column is used to purify acetone to 95%. In contrast, the product mixture of the second case contains acetaldehyde, acetone, ethanol, ethylene, water, CO_2, and H_2. Here, ethylene and acetone are the major components, necessitating separate purification processes. Ethylene purification involves first removing CO_2 using a reactive absorption and stripping column. To achieve 99% purity of ethylene, cryogenic distillation is applied, with refrigerants in the condenser, significantly increasing costs. Meanwhile, purifying acetone to 95% requires the use of more than one distillation column.

The third result pertains to the heat recovery system. In both cases, it is observed that the utility costs are higher for processes without a heat recovery system. This is because, in a heat recovery system, heat exchangers transfer heat between streams, reducing the need for external utilities.

The final result is economic assessment, key economic indicators in case II including NPV, IRR, PI and payback period represent that this case is not interesting to invest according to the complexity of the process is cause to the higher cost in all of the section including capital cost, total raw material cost, total utilities cost, total operating labor cost and total maintenance cost.

5.2 Recommendation

Considering the production process in the second case, using a cooling tower at a low temperature (cryogenic distillation) may not be appropriate. This is because using a utility for the low temperature is refrigerant which cause to the highly cost that making the investment in the second case unfeasible in terms of payback. Further studies might be needed to find other methods that could make the process of producing pure ethylene more attractive for investment.

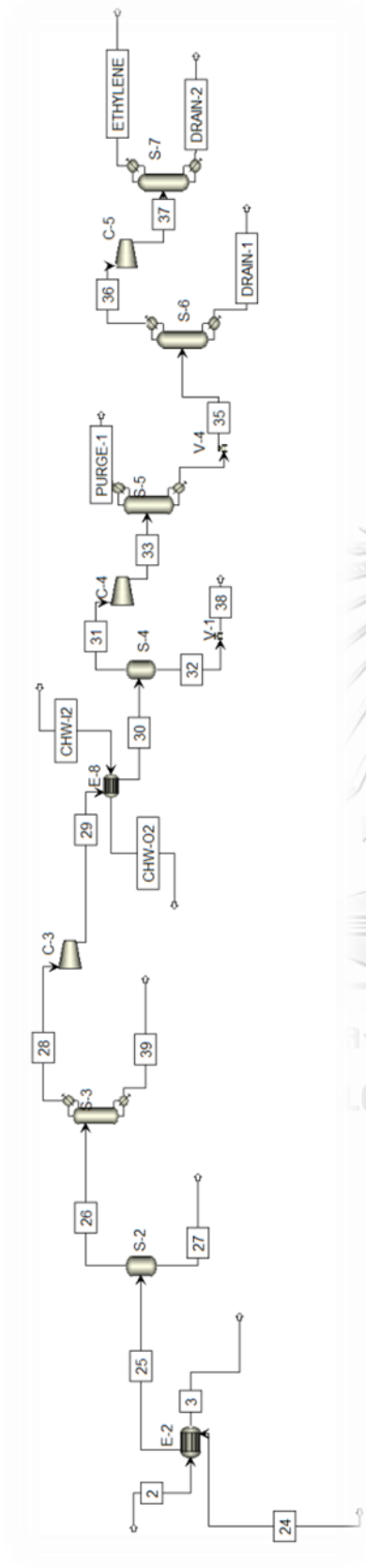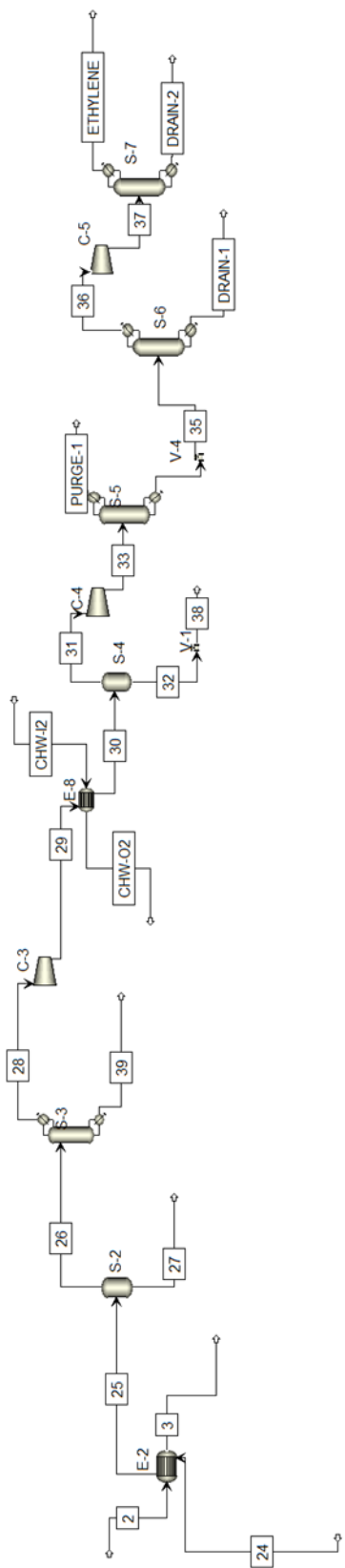Figure 18 Process flow diagram for the cryogenic distillation section in the production of acetone and ethylene from bioethanol.

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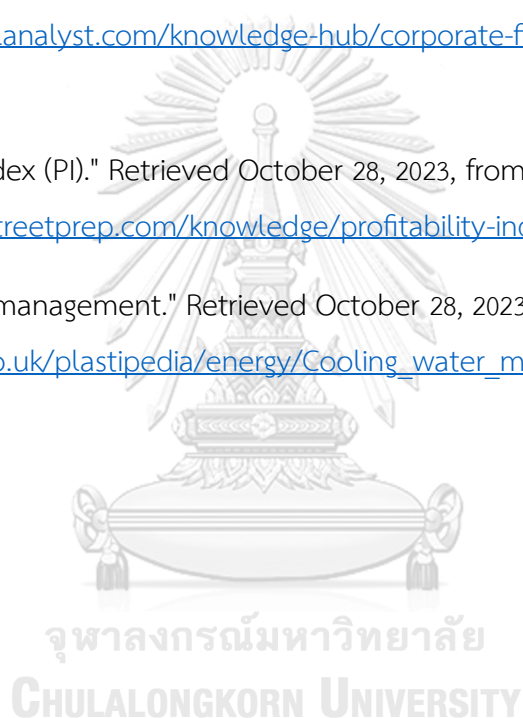
APPENDIX A Calculation of ethanol required and feed amount for acetone production from bioethanol with ZnO-CaO catalyst.

For Acetone production basis in 50,000 tons/year

Ethanol conversion is 1

Yield of ethylene(C_2H_4) is 0.09

Yield of acetone (C_3H_6O) is 0.91

Reaction#1

	C2H5OH	=	C2H4	+	H2O
Mole Stoichiometric	1		1		1
Mass	46		28		18

Reaction#2

	C2H5OH	+	H2O	=	C3H6O +	CO2	+	H2
Mole Stoichiometric2			1		1	1		4
Mass	92		18		58	44		8
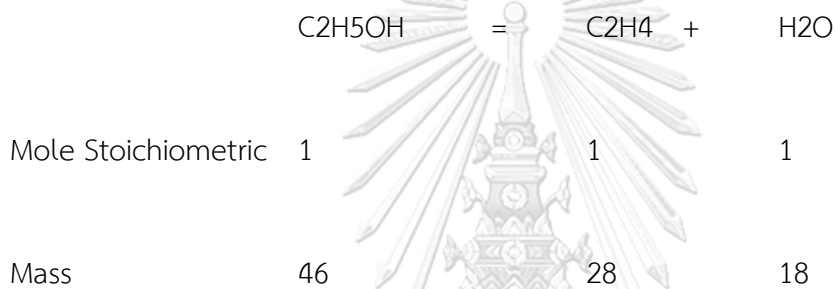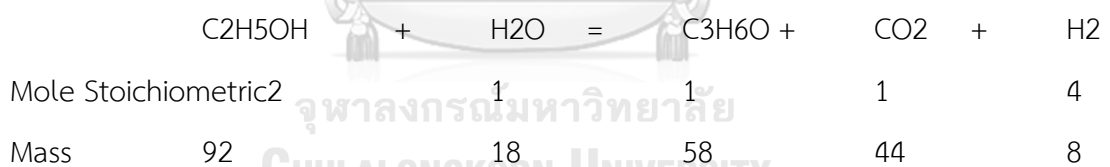
From Reaction#1

C2H4	produced	0.09	mole	C2H5OH	consumed	0.09	mole
				H2O	produced	0.09	mole

From Reaction#2

C3H6O produced	0.455	mole	C2H5OH	consumed	0.91	mole
			H2O	consumed	0.455	mole
			CO2	produced	0.455	mole
			H2	produced	1.82	mole

	CONSUMED		PRODUCED					Feed	
	C2H5OH	H2O	C2H4	H2O	C3H6O	CO2	H2	C2H5OH	H2O
Mole	1	0.455	0.09	0.09	0.455	0.455	1.82	1	4.5597
Mass	46	8.19	2.52	1.62	26.39	20.02	3.64	46	82.0746
Mass/Mass of acetone	1.74	0.31	0.1	0.06	1	0.76	0.14		
Produce 50,000 tons of acetone	87,154.23	15,517.24	4,774.54	3,069.34	50,000	37,931.03	6,896.55		

Ethanol feed is 87, 154.23 tons /year as 36% of feed and 64% of feed is water, the water feed to the reactor is (64% * 87154.23)/36% = 154,940.84 tons/year.

APPENDIX B Reactor sizing

Finding mass flowrate of ethanol with feed (from literature reviews) at 674 K, 0.435 sec, 0.5 g catalyst and 5 ml reactor size

						mole frac
ethanol	1.59	kPa		0.0157	atm	0.1798
water	7.25	kPa		0.0716	atm	0.8202
		sum		0.0873		1

At ethanol

PV   m/MW R T   time   0.435   sec

m   (PVMW)/RT

Where P is 0.0157(0.1798) = 0.0028 atm

   V is 5 ml

   Time 0.435 second

   MW is 46 g/mol

   R is 0.08206 atml/mol K

   T is 674 K

Thus the mass flowrate of ethanol is 2.69859E-05 g/sec

At water, the mass flowrate is 0.000219682 g/sec

Thus the total mass flowrate is 0.000246668 g/sec

From WHSV = $\dfrac{\dot{m}}{W_{cat}}$ where weight of catalyst is 0.5 g

Thus WHSV is 0.000493336 per sec or 1.776009274 per hr

For this simulation results, the mass flowrate to reactor is 25,041.87 kg/hr thus weight of catalyst is 14,100.08 kg or 14.1 tons.

From this study the catalyst ratio between ZnO and CaO is 9:1 by mol

Catalyst ratio ZnO   CaO   9:1 by mol

MW   81.406   56.077

mass   732.654   56.077

Mas ratio   0.93   0.07

From Wcat   14,100.08 kg

Mass (kg)   ZnO   CaO

                13,113.08   987.01

Mass (tons)   13.11307726   0.987005815   is the amount of catalyst for using.

Finding the reactor diameter (D) for packed bed reactor

From $G = \dfrac{4\dot{m}}{\pi D^2}$

Where G is mass velocity in kg/m^2 s

$\dot{m}$ is mass flowrate in kg/hr

D is vessel diameter in m.

From the literature review the total mass flowrate is 0.000246668 g/sec or 0.000888 kg/hr with 4 mm diameter, thus the mass velocity is 70.70100611 kg/m^2 s

From the simulation results assume 4 packed bed reactors.

Thus the mass flowrate of each reactor is 6,260.47 kg/hr with 70.70100611 kg/m^2 s mass velocity, the diameter is 10.62076572 m.

Assume aspect ratio(L/D) is 1.5, thus L or length of packed bed reactor is 15.93 m.

The volume of catalyst bed.

In this work the bulk density of catalyst of ZnO-CaO is 880 kg/m³ and Wcat is 3,525.02 kg/reactor

Catalyst bed volume (V_{bed}) = W_{cat}/bulk density

Thus the catalyst bed volume is 3525.02/880 = 4 m³

The length of bed (L_{bed}) = 4V_{bed}/ πD^2

Thus the length of bed is 0.05 m.

APPENDIX C. Simulation results with heat exchanger recovery

Simulation results of acetone production from bioethanol with ZnO-CaO catalyst with heat exchanger recovery.

	Units	1	2	3	4	5	6	7
From		M-1	E-1	E-2	E-3	E-4	SP-1	SP-1
To		E-1	E-2	E-3	E-4	SP-1	R-1	R-2
Phase		Liquid Phase			Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	79.00	88.62	88.83	229.83	400.00	400.00	400.00
Pressure	bar	1.01	1.01	1.01	1.01	1.01	1.01	1.01
Mass Vapor Fraction		-	0.45	0.46	1.00	1.00	1.00	1.00
Mass Liquid Fraction		1.00	0.55	0.54	-	-	-	-
Mass Flows	kg/hr	25,041.88	25,041.88	25,041.88	25,041.88	25,041.88	6,260.47	6,260.47
ACETONE	kg/hr	-	-	-	-	-	-	-
WATER	kg/hr	16,022.18	16,022.18	16,022.18	16,022.18	16,022.18	4,005.54	4,005.54
ETHANOL	kg/hr	9,019.70	9,019.70	9,019.70	9,019.70	9,019.70	2,254.92	2,254.92
ETHYLENE	kg/hr	-	-	-	-	-	-	-
CO2	kg/hr	-	-	-	-	-	-	-
H2	kg/hr	-	-	-	-	-	-	-

	Units	8	9	10	11	12	13	14
From		SP-1	SP-1	R-1	R-2	R-3	R-4	M-2
To		R-3	R-4	M-2	M-2	M-2	M-2	E-1
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	400.00	400.00	400.00	400.00	400.00	400.00	400.00
Pressure	bar	1.01	1.01	1.01	1.01	1.01	1.01	1.01
Mass Vapor Fraction		1.00	1.00	1.00	1.00	1.00	1.00	1.00
Mass Liquid Fraction		-	-	-	-	-	-	-
Mass Flows	kg/hr	6,260.47	6,260.47	6,260.47	6,260.47	6,260.47	6,260.47	25,041.88
ACETONE	kg/hr	0.00	0.00	1,293.48	1,293.48	1,293.48	1,293.48	5,173.94
WATER	kg/hr	4,005.54	4,005.54	3,683.69	3,683.69	3,683.69	3,683.69	14,734.77
ETHANOL	kg/hr	2,254.92	2,254.92	-	-	-	-	-
ETHYLENE	kg/hr	-	-	123.58	123.58	123.58	123.58	494.33
CO2	kg/hr	-	-	980.13	980.13	980.13	980.13	3,920.52
H2	kg/hr	-	-	179.58	179.58	179.58	179.58	718.32

	Units	15	16	17	18	19	20	21
From		E-1	C-1	E-2	E-3	E-5	E-6	S-1
To		C-1	E-2	E-3	E-5	E-6	S-1	V-1
Phase		Vapor Phase	Vapor Phase	Vapor Phase				Liquid Phase
Temperature	C	90.00	241.65	231.65	101.73	55.79	23.00	23.00
Pressure	bar	1.01	5.07	5.07	5.07	5.07	5.07	5.07
Mass Vapor Fraction		1.00	1.00	1.00	0.48	0.30	0.22	-
Mass Liquid Fraction		-	-	-	0.52	0.70	0.78	1.00
Mass Flows	kg/hr	25,041.88	25,041.88	25,041.88	25,041.88	25,041.88	25,041.88	19,413.70
ACETONE	kg/hr	5,173.94	5,173.94	5,173.94	5,173.94	5,173.94	5,173.94	4,666.07
WATER	kg/hr	14,734.77	14,734.77	14,734.77	14,734.77	14,734.77	14,734.77	14,690.95
ETHANOL	kg/hr	-	-	-	-	-	-	-
ETHYLENE	kg/hr	494.33	494.33	494.33	494.33	494.33	494.33	1.29
CO2	kg/hr	3,920.52	3,920.52	3,920.52	3,920.52	3,920.52	3,920.52	55.18
H2	kg/hr	718.32	718.32	718.32	718.32	718.32	718.32	0.21

	Units	22	23	24	ACETONE	CHW-I	CHW-O	CW-I
From		V-1	S-2	S-2	V-2	E-6	E-6	E-5
To			V-2	V-3		E-6	E-6	E-5
Phase			Liquid Phase	Liquid Phase		Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	22.94	44.89	109.73	44.15	5.00	14.55	30.00
Pressure	bar	1.42	1.22	1.42	1.01	1.01	1.01	1.01
Mass Vapor Fraction		-	-	-	-	-	-	-
Mass Liquid Fraction		1.00	1.00	1.00	1.00	1.00	1.00	1.00
Mass Flows	kg/hr	19,413.70	4,851.01	14,473.70	4,851.01	120,000.00	120,000.00	170,000.00
ACETONE	kg/hr	4,666.07	4,612.26	-	4,612.26	-	-	-
WATER	kg/hr	14,690.95	216.02	14,473.70	216.02	120,000.00	120,000.00	170,000.00
ETHANOL	kg/hr	-	-	-	-	-	-	-
ETHYLENE	kg/hr	1.29	0.41	-	0.41	-	-	-
CO2	kg/hr	55.18	22.31	-	22.31	-	-	-
H2	kg/hr	0.21	-	-	-	-	-	-

Units		CW-O	ETOH-F	PURGE-1	PURGE-2	RECYCLE	WATER-F
From		E-5	M-1	S-1	S-2	V-3	M-1
To							M-1
Phase		Liquid Phase	Liquid Phase	Vapor Phase	Vapor Phase		Liquid Phase
Temperature	C	45.00	30.00	23.00	44.89	100.02	30.00
Pressure	bar	1.01	1.01	5.07	1.22	1.01	1.01
Mass Vapor Fraction		-	-	1.00	1.00	0.02	-
Mass Liquid Fraction		1.00	1.00	-	-	0.98	1.00
Mass Flows	kg/hr	170,000.00	9,494.42	5,628.18	89.03	14,473.70	1,073.76
ACETONE	kg/hr	-	-	507.87	53.86	-	-
WATER	kg/hr	170,000.00	474.72	43.82	1.22	14,473.70	1,073.76
ETHANOL	kg/hr	-	9,019.70	-	-	-	-
ETHYLENE	kg/hr	-	-	493.04	0.88	-	-
CO2	kg/hr	-	-	3,865.34	32.87	-	-
H2	kg/hr	-	-	718.11	0.21	-	-

Simulation results of acetone and ethylene production from bioethanol with ZnO catalyst with heat exchanger recovery.

Reactor Section

	Units	1	2	3	4	5
From		M-1	E-1	E-2	E-3	E-4
To		E-1	E-2	E-3	E-4	FSPLIT-1
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Liquid Phase			Vapor Phase
Temperature	C	34.43	47.95	84.34	93.95	400.00
Pressure	bar	1.01	1.01	1.01	1.01	1.01
Mass Vapor Fraction		-	-	0.14	0.85	1.00
Mass Liquid Fraction		1.00	1.00	0.86	0.15	-
Mass Flows	kg/hr	25,054.28	25,054.28	25,054.28	25,054.28	25,054.28
ETHANOL	kg/hr	9,019.70	9,019.70	9,019.70	9,019.70	9,019.70
WATER	kg/hr	16,034.58	16,034.58	16,034.58	16,034.58	16,034.58
ACETONE	kg/hr	-	-	-	-	-
CO2	kg/hr	-	-	-	-	-
H2	kg/hr	-	-	-	-	-
ACETA-01	kg/hr	-	-	-	-	-
ETHYLENE	kg/hr	-	-	-	-	-
MEA	kg/hr	-	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	6	7	8	9	10
From		FSPLIT-1	FSPLIT-1	FSPLIT-1	FSPLIT-1	R-1
To		R-1	R-2	R-3	R-4	M-2
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	400.00	400.00	400.00	400.00	400.00
Pressure	bar	1.01	1.01	1.01	1.01	1.01
Mass Vapor Fraction		1.00	1.00	1.00	1.00	1.00
Mass Liquid Fraction		-	-	-	-	-
Mass Flows	kg/hr	6,263.57	6,263.57	6,263.57	6,263.57	6,263.57
ETHANOL	kg/hr	2,254.92	2,254.92	2,254.92	2,254.92	31.57
WATER	kg/hr	4,008.65	4,008.65	4,008.65	4,008.65	4,273.82
ACETONE	kg/hr	-	-	-	-	574.62
CO2	kg/hr	-	-	-	-	435.41
H2	kg/hr	-	-	-	-	87.56
ACETA-01	kg/hr	-	-	-	-	170.09
ETHYLENE	kg/hr	-	-	-	-	690.50
MEA	kg/hr	-	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	11	12	13	14	15
From		R-2	R-3	R-4	M-2	E-5
To		M-2	M-2	M-2	E-5	C-1
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	400.00	400.00	400.00	400.00	305.69
Pressure	bar	1.01	1.01	1.01	1.01	1.01
Mass Vapor Fraction		1.00	1.00	1.00	1.00	1.00
Mass Liquid Fraction		-	-	-	-	-
Mass Flows	kg/hr	6,263.57	6,263.57	6,263.57	25,054.28	25,054.28
ETHANOL	kg/hr	31.57	31.57	31.57	126.28	126.28
WATER	kg/hr	4,273.82	4,273.82	4,273.82	17,095.30	17,095.30
ACETONE	kg/hr	574.62	574.62	574.62	2,298.48	2,298.48
CO2	kg/hr	435.41	435.41	435.41	1,741.66	1,741.66
H2	kg/hr	87.56	87.56	87.56	350.24	350.24
ACETA-01	kg/hr	170.09	170.09	170.09	680.34	680.34
ETHYLENE	kg/hr	690.50	690.50	690.50	2,761.98	2,761.98
MEA	kg/hr	-	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	16	17	18	19	20
From		C-1	E-1	E-3	E-6	E-7
To		E-1	E-3	E-6	E-7	S-1
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Vapor Phase	Vapor Phase			
Temperature	C	316.90	293.90	85.90	78.59	75.00
Pressure	bar	1.11	1.11	1.11	1.11	1.11
Mass Vapor Fraction		1.00	1.00	0.61	0.48	0.44
Mass Liquid Fraction		-	-	0.39	0.52	0.56
Mass Flows	kg/hr	25,054.28	25,054.28	25,054.28	25,054.28	25,054.28
ETHANOL	kg/hr	126.28	126.28	126.28	126.28	126.28
WATER	kg/hr	17,095.30	17,095.30	17,095.30	17,095.30	17,095.30
ACETONE	kg/hr	2,298.48	2,298.48	2,298.48	2,298.48	2,298.48
CO2	kg/hr	1,741.66	1,741.66	1,741.66	1,741.66	1,741.66
H2	kg/hr	350.24	350.24	350.24	350.24	350.24
ACETA-01	kg/hr	680.34	680.34	680.34	680.34	680.34
ETHYLENE	kg/hr	2,761.98	2,761.98	2,761.98	2,761.98	2,761.98
MEA	kg/hr	-	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	24	25	43	44	CHW-I	CHW-O
From		C-2	E-2	P-2	E-5	E-7	E-7
To		E-2	S-2	E-5	S-12	E-7	E-7
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Vapor Phase		Liquid Phase		Liquid Phase	Liquid Phase
Temperature	C	259.15	116.32	193.20	307.20	5.00	15.46
Pressure	bar	6.08	6.08	1.11	1.11	1.01	1.01
Mass Vapor Fraction		1.00	0.76	-	0.18	-	-
Mass Liquid Fraction		-	0.24	1.00	0.82	1.00	1.00
Mass Flows	kg/hr	9,679.38	9,679.38	7,309.52	7,309.52	99,916.00	99,916.00
ETHANOL	kg/hr	74.39	74.39	0.24	0.24	-	-
WATER	kg/hr	3,959.75	3,959.75	623.39	623.39	99,916.00	99,916.00
ACETONE	kg/hr	1,716.03	1,716.03	7.57	7.57	-	-
CO2	kg/hr	90.71	90.71	0.02	0.02	-	-
H2	kg/hr	350.24	350.24	-	-	-	-
ACETA-01	kg/hr	601.36	601.36	0.37	0.37	-	-
ETHYLENE	kg/hr	2,604.85	2,604.85	0.07	0.07	-	-
MEA	kg/hr	282.05	282.05	881.34	881.34	-	-
CO3-2	kg/hr	-	-	0.01	0.01	-	-
H3O+	kg/hr	-	-	-	-	-	-
HCO3-	kg/hr	-	-	199.63	199.63	-	-
MEAH+	kg/hr	-	-	2,218.49	2,218.49	-	-
MEACOO-	kg/hr	-	-	3,378.38	3,378.38	-	-
OH-	kg/hr	-	-	-	-	-	-

	Units	CW-I	CW-O	ETOH-F	RECYCLE1	WATER-F
From			E-6			
To		E-6		M-1	M-1	M-1
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	30.00	45.00	30.00	85.61	30.00
Pressure	bar	1.01	1.01	1.01	1.01	1.01
Mass Vapor Fraction		-	-	-	-	-
Mass Liquid Fraction		1.00	1.00	1.00	1.00	1.00
Mass Flows	kg/hr	99,987.00	99,987.00	9,458.09	475.01	15,121.17
ETHANOL	kg/hr	-	-	8,985.19	34.51	-
WATER	kg/hr	99,987.00	99,987.00	472.90	440.50	15,121.17
ACETONE	kg/hr	-	-	-	0.00	-
CO2	kg/hr	-	-	-	-	-
H2	kg/hr	-	-	-	-	-
ACETA-01	kg/hr	-	-	-	-	-
ETHYLENE	kg/hr	-	-	-	-	-
MEA	kg/hr	-	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

Reactive absorption and stripping section

	Units	19	20	21	22	23
From		E-6	E-7	S-1	S-1	ABSORP
To		E-7	S-1	ABSORP	P-3	C-2
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase				Vapor Phase	Liquid Phase	Vapor Phase
Temperature	C	78.59	75.00	75.00	75.00	101.12
Pressure	bar	1.11	1.11	1.11	1.11	1.01
Mass Vapor Fraction		0.48	0.44	1.00	-	1.00
Mass Liquid Fraction		0.52	0.56	-	1.00	-
Mass Flows	kg/hr	25,054.28	25,054.28	10,921.87	14,132.40	9,679.38
ETHANOL	kg/hr	126.28	126.28	93.75	32.53	74.39
WATER	kg/hr	17,095.30	17,095.30	3,393.68	13,701.62	3,959.75
ACETONE	kg/hr	2,298.48	2,298.48	2,068.44	230.04	1,716.03
CO2	kg/hr	1,741.66	1,741.66	1,692.32	49.34	90.71
H2	kg/hr	350.24	350.24	350.24	0.00	350.24
ACETA-01	kg/hr	680.34	680.34	657.38	22.96	601.36
ETHYLENE	kg/hr	2,761.98	2,761.98	2,666.07	95.91	2,604.85
MEA	kg/hr	-	-	-	-	282.05
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	24	39	40	41	42
From		C-2	ABSORP	P-1	STRIPPER	STRIPPER
To		E-2	P-1	STRIPPER	E-9	P-2
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Vapor Phase	Liquid Phase	Liquid Phase	Vapor Phase	Liquid Phase
Temperature	C	259.15	100.88	100.88	136.68	193.20
Pressure	bar	6.08	1.01	1.11	1.01	1.01
Mass Vapor Fraction		1.00	-	-	1.00	-
Mass Liquid Fraction		-	1.00	1.00	-	1.00
Mass Flows	kg/hr	9,679.38	10,054.52	10,054.52	2,745.00	7,309.52
ETHANOL	kg/hr	74.39	19.58	19.58	19.35	0.24
WATER	kg/hr	3,959.75	2,596.46	2,596.46	1,973.07	623.39
ACETONE	kg/hr	1,716.03	359.58	359.58	352.01	7.57
CO2	kg/hr	90.71	29.19	29.19	29.16	0.02
H2	kg/hr	350.24	-	-	-	-
ACETA-01	kg/hr	601.36	56.38	56.38	56.01	0.37
ETHYLENE	kg/hr	2,604.85	61.29	61.29	61.22	0.07
MEA	kg/hr	282.05	1,135.53	1,135.53	254.19	881.34
CO3-2	kg/hr	-	0.01	0.01	-	0.01
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	199.63	199.63	-	199.63
MEAH+	kg/hr	-	2,218.49	2,218.49	-	2,218.49
MEACOO-	kg/hr	-	3,378.38	3,378.38	-	3,378.38
OH-	kg/hr	-	-	-	-	-

	Units	43	44	45	46	47
From		P-2	E-5	S-12	E-9	P-3
To		E-5	S-12	E-9	E-10	M-4
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase		Vapor Phase		Liquid Phase
Temperature	C	193.20	307.20	305.57	145.35	75.12
Pressure	bar	1.11	1.11	1.11	1.11	6.08
Mass Vapor Fraction		-	0.18	1.00	0.97	-
Mass Liquid Fraction		1.00	0.82	-	0.03	1.00
Mass Flows	kg/hr	7,309.52	7,309.52	1,326.70	1,326.70	14,132.40
ETHANOL	kg/hr	0.24	0.24	0.23	0.23	32.53
WATER	kg/hr	623.39	623.39	531.15	531.15	13,701.62
ACETONE	kg/hr	7.57	7.57	7.16	7.16	230.04
CO2	kg/hr	0.02	0.02	0.02	0.02	49.34
H2	kg/hr	-	-	-	-	0.00
ACETA-01	kg/hr	0.37	0.37	0.36	0.36	22.96
ETHYLENE	kg/hr	0.07	0.07	0.07	0.07	95.91
MEA	kg/hr	881.34	881.34	787.72	787.72	-
CO3-2	kg/hr	0.01	0.01	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	199.63	199.63	-	-	-
MEAH+	kg/hr	2,218.49	2,218.49	-	-	-
MEACOO-	kg/hr	3,378.38	3,378.38	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	CHW-I	CHW-O	CW-I2	CW-O2	DRAIN-3
From			E-7		E-10	S-12
To		E-7		E-10		
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	5.00	11.63	30.00	45.00	305.57
Pressure	bar	1.01	1.01	1.01	1.01	1.11
Mass Vapor Fraction		-	-	-	-	-
Mass Liquid Fraction		1.00	1.00	1.00	1.00	1.00
Mass Flows	kg/hr	90,000.00	90,000.00	33,000.00	33,000.00	5,982.82
ETHANOL	kg/hr	-	-	-	-	0.01
WATER	kg/hr	90,000.00	90,000.00	33,000.00	33,000.00	92.25
ACETONE	kg/hr	-	-	-	-	0.41
CO2	kg/hr	-	-	-	-	-
H2	kg/hr	-	-	-	-	-
ACETA-01	kg/hr	-	-	-	-	0.01
ETHYLENE	kg/hr	-	-	-	-	-
MEA	kg/hr	-	-	-	-	93.62
CO3-2	kg/hr	-	-	-	-	0.01
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	199.63
MEAH+	kg/hr	-	-	-	-	2,218.49
MEACOO-	kg/hr	-	-	-	-	3,378.38
OH-	kg/hr	-	-	-	-	-

	Units	PURGE-3	MEA	MEA-F	RECYCLE2	WATER-F2
From		E-9	M-3	M-3	M-3	M-3
To			ABSORP	CONVEN	CONVEN	CONVEN
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	224.68	53.37	35.00	100.34	35.00
Pressure	bar	1.01	1.11	1.11	1.11	1.11
Mass Vapor Fraction		1.00	-	-	-	-
Mass Liquid Fraction		-	1.00	1.00	1.00	1.00
Mass Flows	kg/hr	2,745.00	8,812.03	5,327.47	1,327.35	2,157.21
ETHANOL	kg/hr	19.35	0.23	-	0.23	-
WATER	kg/hr	1,973.07	3,221.47	532.75	531.51	2,157.21
ACETONE	kg/hr	352.01	7.17	-	7.17	-
CO2	kg/hr	29.16	0.02	-	0.02	-
H2	kg/hr	0.00	-	-	-	-
ACETA-01	kg/hr	56.01	0.36	-	0.36	-
ETHYLENE	kg/hr	61.22	0.07	-	0.07	-
MEA	kg/hr	254.19	5,582.70	4,794.72	787.98	-
CO3-2	kg/hr	0.00	-	-	-	-
H3O+	kg/hr	0.00	-	-	-	-
HCO3-	kg/hr	0.00	-	-	-	-
MEAH+	kg/hr	0.00	-	-	-	-
MEACOO-	kg/hr	0.00	-	-	-	-
OH-	kg/hr	0.00	-	-	-	-

Cryogenic distillation section

Units		2	3	24	25	26
From		E-1	E-2	C-2	E-2	S-2
To		E-2	E-3	E-2	S-2	S-3
Phase		Liquid Phase		Vapor Phase		Vapor Phase
Temperature	C	47.95	84.30	259.15	117.02	117.02
Pressure	bar	1.01	1.01	6.08	6.08	6.08
Mass Vapor Fraction		-	0.13	1.00	0.77	1.00
Mass Liquid Fraction		1.00	0.87	-	0.23	-
Mass Flows	kg/hr	25,054.28	25,054.28	9,679.38	9,679.38	7,472.01
ETHANOL	kg/hr	9,019.70	9,019.70	74.39	74.39	68.78
WATER	kg/hr	16,034.58	16,034.58	3,959.75	3,959.75	2,172.09
ACETONE	kg/hr	8.76E-07	8.76E-07	1,716.03	1,716.03	1,649.08
CO2	kg/hr	-	-	90.71	90.71	88.80
H2	kg/hr	-	-	350.24	350.24	350.24
ACETA-01	kg/hr	-	-	601.36	601.36	593.53
ETHYLENE	kg/hr	-	-	2,604.85	2,604.85	2,536.02
MEA	kg/hr	-	-	282.05	282.05	13.48
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	27	28	29	30	31
From		S-2	S-3	C-3	E-8	S-4
To		M-4	C-3	E-8	S-4	C-4
Phase		Liquid Phase	Vapor Phase	Vapor Phase		Vapor Phase
Temperature	C	117.02	-29.64	35.37	6.27	6.27
Pressure	bar	6.08	5.88	15.20	15.20	15.20
Mass Vapor Fraction		-	1.00	1.00	0.93	1.00
Mass Liquid Fraction		1.00	-	-	0.07	-
Mass Flows	kg/hr	2,207.37	3,480.02	3,480.02	3,480.02	3,226.98
ETHANOL	kg/hr	5.62	0.20	0.20	0.20	0.01
WATER	kg/hr	1,787.67	1.35	1.35	1.35	0.11
ACETONE	kg/hr	66.95	165.60	165.60	165.60	55.31
CO2	kg/hr	1.91	88.27	88.27	88.27	87.36
H2	kg/hr	1.60E-05	350.24	350.24	350.24	350.24
ACETA-01	kg/hr	7.83	353.82	353.82	353.82	240.57
ETHYLENE	kg/hr	68.83	2,520.54	2,520.54	2,520.54	2,493.39
MEA	kg/hr	268.56	6.91E-06	6.91E-06	6.91E-06	2.38E-09
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	32	33	34	35	36
From		S-4	C-4	S-5	V-4	S-6
To		V-1	S-5	V-4	S-6	C-5
Phase		Liquid Phase	Vapor Phase	Liquid Phase	Vapor Phase	Vapor Phase
Temperature	C	6.27	22.11	-26.90	-34.73	-33.06
Pressure	bar	15.20	18.95	18.95	15.20	14.19
Mass Vapor Fraction		-	1.00	-	0.07	1.00
Mass Liquid Fraction		1.00	-	1.00	0.93	-
Mass Flows	kg/hr	253.04	3,226.98	2,826.98	2,826.98	2,450.00
ETHANOL	kg/hr	0.19	0.01	0.01	0.01	3.48E-07
WATER	kg/hr	1.23	0.11	0.11	0.11	2.97E-06
ACETONE	kg/hr	110.30	55.31	55.31	55.31	0.08
CO2	kg/hr	0.91	87.36	87.00	87.00	83.78
H2	kg/hr	1.58E-07	350.24	8.41E-19	8.41E-19	-
ACETA-01	kg/hr	113.25	240.57	240.57	240.57	4.44
ETHYLENE	kg/hr	27.15	2,493.39	2,443.99	2,443.99	2,361.69
MEA	kg/hr	6.91E-06	2.38E-09	2.38E-09	2.38E-09	1.58E-16
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	37	38	39	CHW-I2	CHW-O2
From		C-5	V-1	S-3	E-8	E-8
To		S-7	M-4	M-4	E-8	E-8
Phase		Vapor Phase		Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	-31.78	5.96	106.65	5.00	16.15
Pressure	bar	14.49	6.08	6.08	1.01	1.01
Mass Vapor Fraction		1.00	4.41E-08	-	-	-
Mass Liquid Fraction		-	1.00	1.00	1.00	1.00
Mass Flows	kg/hr	2,450.00	253.04	3,992.00	9,000.00	9,000.00
ETHANOL	kg/hr	3.48E-07	0.19	68.57	-	-
WATER	kg/hr	2.97E-06	1.23	2,170.75	9,000.00	9,000.00
ACETONE	kg/hr	0.08	110.30	1,483.48		
CO2	kg/hr	83.78	0.91	0.53		
H2	kg/hr	-	1.58E-07	1.39E-14		
ACETA-01	kg/hr	4.44	113.25	239.71		
ETHYLENE	kg/hr	2,361.69	27.15	15.48		
MEA	kg/hr	1.58E-16	6.91E-06	13.48		
CO3-2	kg/hr	-	-	-		
H3O+	kg/hr	-	-	-		
HCO3-	kg/hr	-	-	-		
MEAH+	kg/hr	-	-	-		
MEACOO-	kg/hr	-	-	-		
OH-	kg/hr	-	-	-	-	-

	Units	DRAIN-1	DRAIN-2	ETHYLENE	PURGE-1
From		S-6	S-7	S-7	S-5
To					
Phase		Liquid Phase	Liquid Phase	Vapor Phase	Vapor Phase
Temperature	C	47.02	-33.6	-41.2	-132.60
Pressure	bar	15.20	14.49	13.98	18.34
Mass Vapor Fraction		-	-	1.00	1.00
Mass Liquid Fraction		1.00	1.00	-	-
Mass Flows	kg/hr	376.98	143.00	2,307.00	400.00
ETHANOL	kg/hr	0.01	3.48E-07	1.79E-54	9.88E-17
WATER	kg/hr	0.11	2.97E-06	2.09E-59	4.23E-14
ACETONE	kg/hr	55.22	0.08	4.94E-36	4.08E-08
CO2	kg/hr	3.22	81.69	2.10	0.36
H2	kg/hr	-	-	-	350.24
ACETA-01	kg/hr	236.12	4.44	2.99E-26	5.03E-06
ETHYLENE	kg/hr	82.29	56.79	2,304.90	49.40
MEA	kg/hr	2.38E-09	-	-	8.68E-27
CO3-2	kg/hr	-	-	-	-
H3O+	kg/hr	-	-	-	-
HCO3-	kg/hr	-	-	-	-
MEAH+	kg/hr	-	-	-	-
MEACOO-	kg/hr	-	-	-	-
OH-	kg/hr	-	-	-	-

Distillation section

	Units	20	21	22	25	26
From		E-7	S-1	S-1	E-2	S-2
To		S-1	ABSORP	P-3	S-2	S-3
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase			Vapor Phase	Liquid Phase	Vapor Phase	Vapor Phase
Temperature	C	75.00	75.00	75.00	116.32	117.02
Pressure	bar	1.11	1.11	1.11	6.08	6.08
Mass Vapor Fraction		0.44	1.00	-	0.76	1.00
Mass Liquid Fraction		0.56	-	1.00	0.24	-
Mass Flows	kg/hr	25,054.28	10,921.87	14,132.40	9,679.38	7,472.01
ETHANOL	kg/hr	126.28	93.75	32.53	74.39	68.78
WATER	kg/hr	17,095.30	3,393.68	13,701.62	3,959.75	2,172.09
ACETONE	kg/hr	2,298.48	2,068.44	230.04	1,716.03	1,649.08
CO2	kg/hr	1,741.66	1,692.32	49.34	90.71	88.80
H2	kg/hr	350.24	350.24	0.00	350.24	350.24
ACETA-01	kg/hr	680.34	657.38	22.96	601.36	593.53
ETHYLENE	kg/hr	2,761.98	2,666.07	95.91	2,604.85	2,536.02
MEA	kg/hr	-	-	-	282.05	13.48
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	27	28	29	30	31
From		S-2	S-3	C-3	E-8	S-4
To		M-4	C-3	E-8	S-4	C-4
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Vapor Phase	Vapor Phase		Vapor Phase
Temperature	C	117.02	-29.64071277	35.37	7.89	6.27
Pressure	bar	6.08	5.88	15.20	15.20	15.20
Mass Vapor Fraction		-	1.00	1.00	0.93	1.00
Mass Liquid Fraction		1.00	-	-	0.07	-
Mass Flows	kg/hr	2,207.37	3,480.02	3,480.02	3,480.02	3,226.98
ETHANOL	kg/hr	5.62	0.20	0.20	0.20	0.01
WATER	kg/hr	1,787.67	1.35	1.35	1.35	0.11
ACETONE	kg/hr	66.95	165.60	165.60	165.60	55.31
CO2	kg/hr	1.91	88.27	88.27	88.27	87.36
H2	kg/hr	0.00	350.24	350.24	350.24	350.24
ACETA-01	kg/hr	7.83	353.82	353.82	353.82	240.57
ETHYLENE	kg/hr	68.83	2,520.54	2,520.54	2,520.54	2,493.39
MEA	kg/hr	268.56	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	32	37	38	47	48
From		S-4	V-1	S-3	P-3	M-4
To		V-1	M-4	M-4	M-4	S-8
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase		Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	6.27	5.96	106.65	75.12	85.10
Pressure	bar	15.20	6.08	6.08	6.08	6.08
Mass Vapor Fraction		-	0.00	-	-	-
Mass Liquid Fraction		1.00	1.00	1.00	1.00	1.00
Mass Flows	kg/hr	253.04	253.04	3,992.00	14,132.40	20,584.81
ETHANOL	kg/hr	0.19	0.19	68.57	32.53	106.91
WATER	kg/hr	1.23	1.23	2,170.75	13,701.62	17,661.27
ACETONE	kg/hr	110.30	110.30	1,483.48	230.04	1,890.76
CO2	kg/hr	0.91	0.91	0.53	49.34	52.69
H2	kg/hr	-	-	-	6.53E-06	-
ACETA-01	kg/hr	113.25	113.25	239.71	22.96	383.75
ETHYLENE	kg/hr	27.15	27.15	15.48	95.91	207.37
MEA	kg/hr	-	-	13.48	-	282.05
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	49	50	51	52	ACETONE
From		S-8	S-9	V-2	S-10	S-10
To		S-9	V-2	S-10	V-3	S-10
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Liquid Phase		Liquid Phase	Liquid Phase
Temperature	C	142.66	107.45	64.05	98.24	56.37
Pressure	bar	6.08	5.07	1.22	1.22	1.01
Mass Vapor Fraction		-	-	0.20	-	-
Mass Liquid Fraction		1.00	1.00	0.80	1.00	1.00
Mass Flows	kg/hr	19,924.49	2,455.01	2,455.01	475.01	1,980.00
ETHANOL	kg/hr	106.89	106.89	106.89	33.83	73.06
WATER	kg/hr	17,656.68	469.24	469.24	441.18	28.06
ACETONE	kg/hr	1,878.59	1,878.60	1,878.60	-	1,878.60
CO2	kg/hr	-	-	-	-	-
H2	kg/hr	-	-	-	-	-
ACETA-01	kg/hr	-	-	-	-	-
ETHYLENE	kg/hr	0.27	0.27	0.27	-	0.27
MEA	kg/hr	282.05	-	-	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

	Units	CHW-I2	CHW-O2	DRAIN-4	PURGE-2	RECYCLE1
From			E-8	S-9	S-8	
To		E-8				M-1
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase	Liquid Phase
Temperature	C	5.00	16.65	159.61	51.29	85.61
Pressure	bar	1.01	1.01	6.08	5.07	1.01
Mass Vapor Fraction		-	-	-	1.00	-
Mass Liquid Fraction		1.00	1.00	1.00	-	1.00
Mass Flows	kg/hr	8,000.00	8,000.00	17,469.49	660.32	475.01
ETHANOL	kg/hr	-	-	-	0.02	34.51
WATER	kg/hr	8,000.00	8,000.00	17,187.44	4.59	440.50
ACETONE	kg/hr	-	-	-	12.17	-
CO2	kg/hr	-	-	-	52.69	-
H2	kg/hr	-	-	-	-	-
ACETA-01	kg/hr	-	-	-	383.75	-
ETHYLENE	kg/hr	-	-	-	207.10	-
MEA	kg/hr	-	-	282.05	-	-
CO3-2	kg/hr	-	-	-	-	-
H3O+	kg/hr	-	-	-	-	-
HCO3-	kg/hr	-	-	-	-	-
MEAH+	kg/hr	-	-	-	-	-
MEACOO-	kg/hr	-	-	-	-	-
OH-	kg/hr	-	-	-	-	-

VITA

NAME	Thanyarath Nueangchamnong
DATE OF BIRTH	3 October 1994
PLACE OF BIRTH	Chonburi
INSTITUTIONS ATTENDED	Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University
HOME ADDRESS	99/320 Ban-puek sub-district Chonburi 20130

จุฬาลงกรณ์มหาวิทยาลัย

CHULALONGKORN UNIVERSITY