Techno-Economic Analysis of Acetaldehyde Production via Partial Oxidative Dehydrogenation of Ethanol

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การวิเคราะห์ทางเศรษฐศาสตร์และเทคโนโลยีของกระบวนการผลิตอะเซทัลดีไฮด์ผ่านปฏิกิริยาออกซิเดทีฟดีไฮโดรจิเนชันเพียงบางส่วนของเอทานอล

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เนื่องจากความสนใจที่เพิ่มขึ้นเกี่ยวกับรถยนต์ไฟฟ้าแบตเตอรี่ (BEV) เป็นผลให้ความต้องการเอทานอลเพื่อใช้เป็นเชื้อเพลิงชีวภาพอาจลดลงได้ในอนาคต ดังนั้นการเปลี่ยนรูปเอทานอลเป็นอะเซทัลดีไฮด์จึงถูกดำเนินการในงานวิจัยนี้ ทั้งนี้เพราะราคาที่สูงกว่าและประโยชน์ที่หลากหลายของอะเซทัลดีไฮด์ โดยการผลิตอะเซทัลดีไฮด์จะผลิตผ่านปฏิกิริยาออกซิเดทีฟดีไฮโดรจิเนชันเพียงบางส่วนของเอทานอล

จากผลการวิเคราะห์ทางเศรษฐศาสตร์พบว่าที่ราคาอะเซทัลดีไฮด์เดียวกันกำลังการผลิตที่ 120,000 ตันต่อปีเป็นขนาดการผลิตที่ให้ผลกำไรสูงที่สุด นอกจากนี้กระบวนการที่มีศักยภาพในการผลิตอะซีทัลดีไฮด์จากเอทานอลคือกระบวนการผลิตอะเซทัลดีไฮด์ที่อุณหภูมิ 200°C เพราะกระบวนการนี้ให้ระยะเวลาคืนทุน (POP) ที่สั้นกว่าและอัตราผลตอบแทนภายใน (IRR) ที่สูงกว่าเมื่อเทียบกับอีกกระบวนการหนึ่งนั่นคือกระบวนการผลิตอะเซทัลดีไฮด์ที่อุณหภูมิ 300°C ในเรื่องการใช้พลังงานกระบวนการที่ดำเนินการที่อุณหภูมิ 200°C ใช้สาธารณูปโภคทางความร้อนมากกว่าที่อุณหภูมิ 300°C เนื่องจากปฏิกิริยาให้ค่าเปอร์เซ็นต์การเปลี่ยนแปลงวัตถุดิบไปเป็นผลิตภัณฑ์ต่ำและด้วยเหตุผลเดียวกันยังทำให้การปล่อยก๊าซคาร์บอนไดออกไซด์ในกรณีของการดำเนินการที่ 200°C ออกมามากกว่าเช่นกัน สำหรับการใช้สาธารณูปโภคทางไฟฟ้ากระบวนการที่ดำเนินการที่อุณหภูมิ 300°C มีปริมาณการใช้ไฟฟ้ามากกว่าเพราะมีคอมเพรสเซอร์ถูกใช้ในกระบวนการ ซึ่งการมีอยู่ของคอมเพรสเซอร์ก็เป็นสาเหตุหนึ่งที่ทำให้กระบวนการนี้ได้กำไรน้อยลง

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Sudarat Sompong : Techno-Economic Analysis of Acetaldehyde Production via Partial Oxidative Dehydrogenation of Ethanol. Advisor: Pongtorn Charoensuppanimit, Ph.D. Co-advisor: Prof. BUNJERD JONGSOMJIT, Ph.D.

Due to the increased attention regarding the battery electric vehicles, the demand for ethanol as a biofuel may be reduced in the future. Therefore, ethanol transformation towards acetaldehyde is conducted in this work, primarily because of the higher selling price and several advantages of acetaldehyde. Regarding the acetaldehyde preparation, acetaldehyde is produced by partial oxidative dehydrogenation of ethanol.

According to the economic analysis results, at the same price of acetaldehyde, an annual production capacity of 120,000 tons is the most profitable production size. In addition, the potential process of producing acetaldehyde from ethanol is acetaldehyde production process at 200°C since this process offers a shorter POP and a higher IRR compared to another process, namely acetaldehyde production process at 300°C. For energy consumption, the process performed at temperature of 200°C requires more thermal utilities than that of 300°C. This is because the low conversion of ethanol. For the same reason, the CO_2 emissions in the case of operating at 200°C are also higher. Regarding the usage of electric utilities, the process performed at 300°C consumes the higher amount of electricity since a gas compressor is used in the process. The existence of this compressor is one of the reasons that makes this process less profitable.

Field of Study:	Chemical Engineering	Student's Signature ....
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TABLE OF CONTENTS

Page

LIST OF TABLES

LIST OF FIGURES

CHAPTER I

INTRODUCTION

1.1 Background

Over the years, fossil fuels are generally used to produce energy. However, the fossil fuels are depletable since they are non-renewable that cannot be replenished to match the energy consumption of human. In addition, the burning of fossil fuels results in the production of carbon dioxide, sulfur dioxide, and nitrogen oxides that impact the environment and human. Therefore, the renewable energy is considered as the alternative to fossil fuels since it is generated from natural resources such as biomass, wind, sunlight or water that can be constantly replaced and eco-friendly [1].

Bioethanol is one of the biomass products that can be produced by the fermentation of starch or sugar crops. It can be used as a mixture in fuel for vehicles or as a starting material for the chemical industries such as acetaldehyde, isobutylene ethyl acetate, acetic acid, and others [2].

In Thailand, the domestic raw materials from agricultural crops such as molasses, cane juice, and cassava are used in the production of ethanol. Ethanol produced is then used as a fuel additive for gasohol (i.e., E10, E20, and E85), a greener fuel used in vehicles [3]. When gasoline blends with ethanol, contributing to the decreasing of carbon dioxide concentrations in the atmosphere compared to traditional gasoline [4, 5].

However, electrical vehicles (EV) with the advancement in battery technology have gained increased attentions due to its environmentally friendliness and its saving on fuel and maintenance costs compared to the conventional internal combustion engine cars (ICE) [6].

Table 1. Global Automobile Sales (units)

Year	ICE+HEV	% Growth	PHEV+ BEV	% Growth	Total	% Growth	% share of EV (PHEV+BEV)
2011	78,149,440	4.2	48,160	634.1	78,197,600	4.3	0.06
2012	82,047,695	5.0	118,690	146.4	82,166,385	5.1	0.14
2013	85,450,098	4.1	192,010	61.8	85,642,108	4.2	0.22
2014	87,595,058	2.5	325,090	69.3	87,920,148	2.7	0.37
2015	89,127,413	1.8	550,570	69.4	89,677,983	2	0.61
2016	**93,074,579**	**4.4**	**781,809**	**42.0**	**93,856,388**	**4.7**	**0.83**

As seen in Table 1, sales of PHEV and HEV in 2016 are estimated to be about 0.78 million vehicles which account for only 0.83% of the total automobile sales. Nevertheless, the sales growth rate of PHEV and BEV (42%) is approximately 10 times greater than that of ICE and HEV (4.4%) [7]. It exhibits that electric vehicles may replace the current automotive technology. As such, the ethanol demand for gasohol may decrease in the future.

Therefore, the use of ethanol as a precursor to produce higher valued chemical such as acetaldehyde is a potential way for the bioethanol utilization due to its several advantages including; 1) Acetaldehyde is more expensive than ethanol; 2) Acetaldehyde has a wide range of applications such as a food preservative, as a flavoring agent, and as an intermediate for producing acetic acid, 1,3-butylene glycol, pentaerythritol, ethyl acetate, pyridine, crotonaldehyde, acetic anhydride, peracetic acid and many other chemicals [8]. According to the world consumption of acetaldehyde in 2016, the chemicals produced from acetaldehyde are divided into 4 major groups including pyridines, pentaerythritol, acetic acid, and acetate esters, which account for 34%, 23%, 18%, and 10%, respectively, of total production [9].

Typically, the main chemical reactions for acetaldehyde productions from ethanol include dehydrogenation and partial oxidative dehydrogenation reactions. Provided the lower operating temperature and less coke formation on the catalyst compared to another method [10], the partial oxidative dehydrogenation reaction was chosen for process analysis and economic evaluation in this work.

In this work, two different data sets obtained from oxidative dehydrogenation of ethanol to produce acetaldehyde using V-Zr-La/SBA-15 catalyst are used to simulate by a process simulator, namely Aspen plus. As we know, the use of different operating conditions in chemical reaction gives different results, for instance; conversion, selectivity, yield and by-products. In the laboratory, the catalysis research groups are only interested in terms of maximized conversion and product selectivity. However, the difficulty in separating of by-products that occur never take into consideration. The presence of several by-products may affect the design of separation system, energy demand for separating each component as well as capital investment. Thus, the process design and simulation are performed to analyze these things in this work. After that, techno-economic analysis of the simulated processes is to be determined. The simulation and techno-economic results provided herein are compared to select the appropriate manufacturing process for an acetaldehyde product and to prove the feasibility of this ethanol valorization process via acetaldehyde production which may suggest an alternative way of utilizing ethanol in the future.

1.2 Objective

The aim of this work is to simulate processes for acetaldehyde production via oxidative dehydrogenation of ethanol over V-Zr-La/SBA-15 catalyst based on data from literatures, leading to the economic evaluation of the simulated processes using Aspen Plus. Finally, the results of each process will be compared to identify the appropriate process for the production of acetaldehyde.

1.3 Scope of work

1.3.1 The oxidative dehydrogenation reaction is utilized to produce acetaldehyde.

1.3.2 Ethanol and oxygen obtained from the atmosphere are used as reactants.

1.3.3 The influences of different operating conditions in oxidative dehydrogenation of ethanol over V-Zr-La/SBA-15 catalyst on process performance such as process profitability, energy consumptions and CO_2 emissions are to be examined. The conditions investigated in this work are as follows:

- At reaction temperature of 300 °C and atmospheric pressure.
- At reaction temperature of 200 °C and atmospheric pressure.

1.3.4 Aspen Plus is used to simulate the proposed process and to evaluate the economics of acetaldehyde production process.

1.4 Expected benefits

Process simulation of acetaldehyde production via the vapor phase oxidation of ethanol contributes to the insights regarding factors affecting the performance of acetaldehyde production such as process profitability, energy efficiency of the process and CO_2 emissions. These factors include process variables such as raw material, conversion and product selectivity, operating condition, energy consumption (especially in the separation units), and raw material and product prices. Attainment of the key factors would benefit the chemical industry since this could provide recommendation regarding the design of acetaldehyde production from ethanol.

CHAPTER II

FUNDAMENTALS AND LITERATURE REVIEWS

The summary information related to ethanol, acetaldehyde, oxidative dehydrogenation reaction, input data and methods of azeotropic mixture separation used for simulating acetaldehyde production process in this work is provided in Chapter 2.

2.1 Fundamentals

2.1.1 Ethanol

Ethanol, also known as ethyl alcohol, is the major fermentation product from renewable biomass, the green chemical that has recently received considerable attention to decrease carbon emissions from fossil fuels. As a result, biomass-based ethanol that is economical alternative usage method is introduced.

Regarding the utilization of ethanol, ethanol is also considered as a versatile building block for bio-refinery as illustrated in Figure 1. This figure represents the direct production of chemicals from ethanol that is a new opportunity for the transformation of ethanol into valuable products such as acetaldehyde, hydrogen, acetic acid, ethylene, etc. [2].

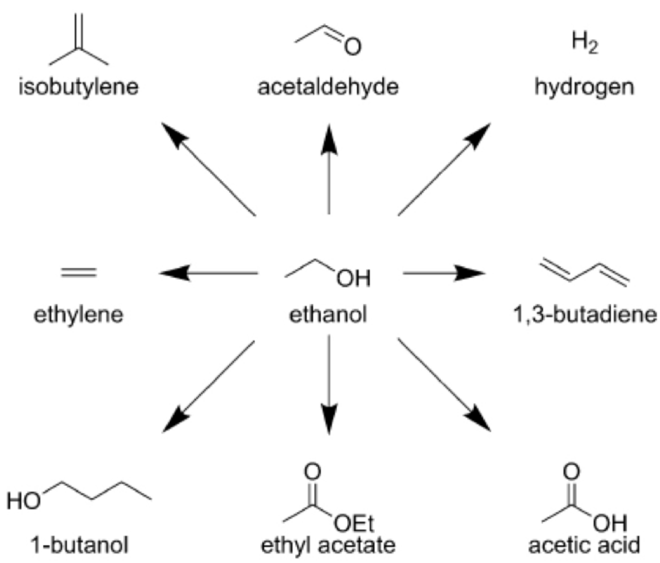


Figure 1. Examples of chemicals derive from ethanol conversion

In general, ethanol is a colorless liquid. Physical and chemical properties of ethanol are listed in Table 2 [11, 12].

Table 2. Physical and chemical properties of ethanol

Properties	Ethanol
Melting point	-114 °C
Boiling point	78 °C
Critical temperature	241±7 °C
Vapor pressure	44.6 mmHg at 20 °C
Solubility	Easily soluble in water
Flash point	14 °C
Flammability	Flammable liquid
Auto-ignition temperature	363 °C
Explosive limit - Lower	3.3 %V
Explosive limit - Upper	19.0 %V

2.1.2 Acetaldehyde

Acetaldehyde is sometimes called ethanal containing a functional group -CHO. Its chemical formula can be written as CH_3CHO. At room temperature, the appearance of acetaldehyde is a colorless liquid with a pungent odor. Physical and chemical properties of acetaldehyde are shown in Table 3 [13, 14].

Table 3. Physical and chemical properties of acetaldehyde

Properties	Acetaldehyde
Melting point	-123 °C
Boiling point	20.4 °C
Critical temperature	193 °C
Vapor pressure	1.006 hPa at 20 °C
Solubility	Easily soluble in water
Flash point	-20 °C
Flammability	Flammable liquid
Auto-ignition temperature	> 400 °C
Explosive limit - Lower	4.0 %V
Explosive limit - Upper	57.0 %V

There are four common methods used for the production of acetaldehyde from various types of raw materials including:

- Oxidation of ethylene

In the 1950s, ethylene oxidation over $PdCl_2$ and $CuCl_2$ catalysts, commonly known as the Wacker process, has been discovered to produce acetaldehyde [15]. The catalytic reaction is provided in the following steps.

The 1st step: ethylene and $PdCl_2$ are reacted to form acetaldehyde and Pd(0).

$$C_2H_4 + PdCl_2 + H_2O \longrightarrow CH_3CHO + Pd^0 + 2HCl \quad (1)$$

The 2nd step: cupric chloride ($CuCl_2$) reoxidizes Pd(0) into Pd(II).

$$Pd^0 + 2CuCl_2 \longrightarrow PdCl_2 + Cu_2Cl_2 \quad (2)$$

The 3rd step: cuprous chloride (Cu_2Cl_2) is reoxidized to the cupric state with O_2.

$$Cu_2Cl_2 + 2HCl + 0.5O_2 \longrightarrow 2CuCl_2 + H_2O \quad (3)$$

Overall:

$$C_2H_4 + 0.5O_2 \longrightarrow CH_3CHO \quad (4)$$

- Hydration of acetylene

Prior to the Wacker process, acetaldehyde is produced from acetylene reacted with water in the presence of acid catalysts such as mercury salt in acidic aqueous solution. The acetylene hydration reaction is given in the equation below [16].

$$C_2H_2 + H_2O \xrightarrow[H^+]{Hg^{2+}} CH_3CHO \quad (5)$$

- Non-oxidative dehydrogenation of ethanol

Non-oxidative dehydrogenation of alcohol is one of the important reactions for aldehyde compound production that involves the removal of two hydrogen atoms from an alcohol molecule and forms a molecule containing a double bond between a carbon atom and an oxygen atom (C=O), which usually represents the desired product.

For the non-oxidative dehydrogenation of ethanol, 1 moles of ethanol are used to generate 1 mole of acetaldehyde and 1 mole of hydrogen as shown in Eq. (6), making it an endothermic reaction [17].

$$C_2H_5OH \longrightarrow CH_3CHO + H_2 \quad (6)$$

- Oxidative dehydrogenation of ethanol

Oxidative dehydrogenation means the formation of water by contacting of an organic molecule and oxygen during the chemical reaction.

In the case of oxidative dehydrogenation of ethanol, the reaction is an exothermic reaction which will be dehydrogenated in the presence of molecular oxygen through a suitable catalyst to form acetaldehyde and water as a by-product. The reaction is given in the following equation [17].

$$C_2H_5OH + 0.5O_2 \longrightarrow CH_3CHO + H_2O \quad (7)$$

Ethanol is classified as a primary alcohol (RCH_2OH), used to prepare aldehydes via oxidative dehydrogenation reaction. However, if a secondary alcohol is used instead of a primary alcohol, the reaction product is a ketone. Eq. (8) represents the transformation of secondary alcohols to ketones [18].

$$RCHOHR' + 0.5O_2 \xrightarrow{catalyst} R\text{-}CO\text{-}R' + H_2O \quad (8)$$

Table 4. A comparison between non-oxidative and oxidative dehydrogenation of ethanol to produce acetaldehyde

Non-oxidative dehydrogenation of ethanol	**Oxidative dehydrogenation of ethanol**
Endothermic reaction	Exothermic reaction
Advantages - Environmental friendliness - Receiving hydrogen as a by product	**Advantages** - Low operating temperature - Less coke formation
Disadvantages - Operating at higher temperature that contribute to the catalyst deactivation and coke formation	**Disadvantages** - CO_2 can be generated

As seen in Table 4, although oxidative dehydrogenation of ethanol may produce carbon dioxide releasing into the atmosphere, but it has a lower operating temperature and coke formation compared to another method, namely non-oxidative dehydrogenation of ethanol. In this work, the oxidative dehydrogenation reaction is therefore chosen for these reasons.

2.2 Literature reviews

This section reviews the literatures concerning the production of acetaldehyde via oxidative dehydrogenation of ethanol.

2.2.1 Catalysts and reaction involved in acetaldehyde productions

According to Section 2.1.2, acetaldehyde can be produced by various methods. Regarding the oxidation of ethylene, this reaction is recognized by advantages such as the small amount of $PdCl_2$ required for the reaction and regeneration of the spent catalyst. Nevertheless, the process economic is quite a problem because 1) the requirement of using special materials for corrosion resistance, and 2) waste-air purification and wastewater treatment are required to eliminate chlorocarbon, which have a high acute toxicity that affect on living organisms, the disadvantages of this reaction [19]. For the hydration of acetylene, the catalyst used in the process is mercury salts in acidic solution, which is toxic and dangerous.

Non-oxidative dehydrogenation of ethanol has emerged as an alternative route because of its desired attributes such as its process economic and its environmental friendliness [20]. Nevertheless, this reaction needs to operate at high temperature and results in coke formation, contributing to catalyst deactivation. On the other hand, the production of acetaldehyde via oxidative dehydrogenation of ethanol seems highly attractive since the reaction can perform at lower temperature and less coke deposition on the catalyst in the presence of oxygen [10]. Furthermore, due to the involvement of battery electric vehicles, low cost and availability of ethanol, the transformation of ethanol towards acetaldehyde is therefore considered to be a high-quality raw material. Accordingly, acetaldehyde production via oxidative dehydrogenation of ethanol is chosen for process analysis and economic evaluation in this work.

Further, regarding the use of experimental results as input data to apply them in the simulation, the simulation data are obtained from the literatures depending on the parameters involved in the process, for instance; conversion, selectivity, yield, by-products and operating conditions. Various types of catalyst under different conditions to produce acetaldehyde from gas-phase oxidation of ethanol are listed in Table 5.

Table 5. Various catalysts used in ethanol oxidative dehydrogenation to acetaldehyde

Catalyst	Temperature (°C)	Pressure (atm)	Ethanol Conversion (%)	Acetaldehyde Selectivity (%)	Acetaldehyde Yield (%)	Ref.
V/Al_2O_3	250	1	51.21	65.98	33.79	[19]
Mg-Al-450	350	1	45.80	64.90	29.72	[21]
Au/ZrO_2	350	5	38	72	27.36	[22]
Ag/CeO_2	350	5	36	87	31.32	[23]
V-Zr-La/ SBA-15	300	1	98	41	40	[20]
Ag/HAp	277	1	18	100	18	[24]

According to the table, since the V-Zr-La/SBA-15 (vanadium oxide doped in SBA-15 supported catalyst with Zr and La modification) gives the maximum ethanol conversion with the maximum acetaldehyde yield at reaction temperature of 300°C and atmospheric pressure, the V-Zr-La/SBA-15-HT is preferred to produce acetaldehyde when compared to other catalysts. The main reaction that takes place is provided in the following equation.

$$C_2H_5OH + 0.5O_2 \longrightarrow CH_3CHO + H_2O \quad (9)$$

Meanwhile, the four main by-products are also produced including carbon dioxide, carbon monoxide, ethylene and diethyl ether (DEE), which is represented as follows:

$$C_2H_5OH + 3O_2 \longrightarrow 2CO_2 + 3H_2O \quad (10)$$

$$C_2H_5OH + 2O_2 \longrightarrow 2CO + 3H_2O \quad (11)$$

$$C_2H_5OH \longrightarrow C_2H_4 + H_2O \quad (12)$$

$$2C_2H_5OH \longrightarrow C_2H_5OC_2H_5 + H_2O \quad (13)$$

Besides, ethanol oxidative dehydrogenation under the same type of catalyst (namely V-Zr-La/SBA-15) at operating temperature of 200°C and atmospheric pressure giving 11% conversion of ethanol and 99% selectivity of acetaldehyde is also performed for comparative purpose. Since each condition has its own advantages and disadvantages, the process designs obtained according to each process are undertaken which are useful for the recommendations to the prospective producers of acetaldehyde. This is again consistent with the objective of this work. Therefore, as mentioned above, two sets of experimental data obtained from catalytic oxidation of ethanol using V-Zr-La/SBA-15 catalyst under different operating conditions are determined for process simulation and economic analysis, leading to comparative studies of these two processes in this work. This experimental results of these two processes such as conversion and selectivity are summarized in Table 6.

Table 6. Summary results of different operating condition in oxidative dehydrogenation of ethanol using V-Zr-La/SBA-15 catalyst

T (°C)	P (atm)	Ethanol conversion (%)	Selectivity (%)				
			Acetaldehyde	DEE	CO_2	CO	C_2H_4
200	1	11	99	1	-	-	-
300	1	98	41	1	21.5	21.5	15

2.2.2 Separation of problematic side-products

As mentioned that different conditions yield different side products. Some side products cause problem to the process particularly in the separation units. For example, azeotropic mixtures that are expected in this process including water/ethanol and acetaldehyde and DEE.

Due to the presence of water in the process, the azeotropic mixture of ethanol-water is formed. As such, the high purity ethanol product cannot be altered by conventional distillation technique because of the azeotropic point. Thus, the enhanced techniques for eliminating the azeotrope are necessary, which is explained as follows:

- Pressure-swing distillation (PSD)

For the process having a pressure sensitive azeotrope, pressure-swing distillation can be used to obtain pure components. The main advantage of pressure-swing distillation process is that the addition of a separating agent does not require. Additionally, the heat integration in continuous process is possible to be conducted which can conserve energy [25]. To separate ethanol from water by this technique, the change in the composition of ethanol-water mixtures at different pressure has been proposed in accordance with the figure below.

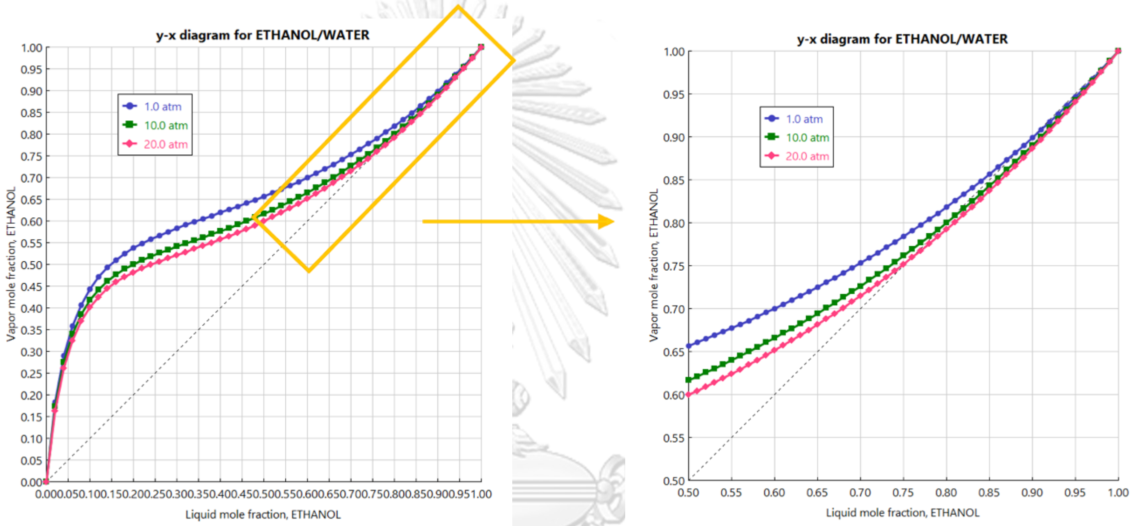


Figure 2. Binary x-y diagram of ethanol-water mixture at different pressure using NRTL-RK model

As depicted in Figure 2, we can notice that the pressure sensitivity of ethanol-water binary mixture is changed relatively low. Nonetheless, there are some researches that perform the ethanol dehydration using pressure-swing distillation process. Iqbal and Ahmad [26] reported that pressure-swing distillation could be applied to ethanol-water azeotrope based on their simulation by Aspen Plus. In the literature, 99.7 mol% of ethanol concentration was received at operating pressures of 1 atm for low pressure column and 10 atm for high pressure column. However, the drawback of pressure-swing distillation is that the high-pressure column may have a relatively high cost to maintain the condition in the column.

- Pervaporation

Pervaporation is used to separate azeotropic mixture as well, which is associated with the membrane usage. Regarding the procedure, a binary liquid mixture is fed to contact with one side of the membrane that sorption of permeating component occurs before diffusion through the membrane. Finally, in the permeate side of the membrane, a selective component is formed in a vapor state. This technique presents several advantages including; 1) the low separation energy is required; 2) the membrane process can be processed at room temperature, therefore, suitable to separate heat-sensitive components; and 3) there is no additional a third component. However, the problem concerning the membrane stability may be the limitation of this technique [27].

- Extractive distillation

By application, extractive distillation is a method where a separating agent, so called an entrainer, is introduced into the system to separate azeotropes or close boiling components by increasing the relative volatility. The required properties of the entrainer for this technique are miscible and have a high boiling point.

The principle of this method starts with loading the entrainer close to the top and the azeotropic mixture at few stages below the entrainer feed stage of the first extraction column. The overhead product of this column is the light key component with a high purity, while the bottom consisting of the entrainer and another component is fed to the recovery column where the entrainer is retrieved and then recycle back to the first column. Please note that the entrainer must not be formed an azeotrope with any components in the original mixture [28].

From all of the above separation techniques, this work focuses on the extractive distillation. The reason is that:

1) Ghuge et al. [29] had performed a comparative study of extractive and pressure-swing distillation to separate tetrahydrofuran-water azeotrope. The result indicated that the total annual cost (TAC) and total energy consumption of extractive distillation were lower than that of pressure-swing distillation. Similar results were reported by Luyben that studied in

the cases of separating acetone-chloroform [30] and acetone-methanol azeotrope [31]. Thus, extractive distillation appears to be more economical as compared to pressure-swing distillation process.

2) The most of the membranes used for pervaporation are made from polymer. Thus, pervaporation can’t perform at high temperature compared to extractive distillation process since the membrane decomposition may be occurred.

Table 7 represents a list of entrainers used for each binary system [32]. According to the table, two entrainers can be used for eliminating ethanol-water azeotrope including ethylene glycol and glycerine.

Table 7. The recommend entrainer for extractive distillation

Mixture	Entrainer
Butadiene/Butene from C4 fractions	Furfural, Acetonitrile, NMP, DMF
Butane/Butene	Acetone
Butene/Isoprene	DMF
Acetone/Methanol	Water, Aniline, Ethylene glycol
Ethanol/Water	Ethylene glycol, Glycerine
Benzene/Cyclohexane	Aniline
Toluene/Heptane	Aniline, Phenol
Propylene/Propane	Acrylonitrile
HCl/Water, Nitric acid/Water	Sulfuric acid
Tetrahydrofuran/Water	DMF, Propylene glycol
Cumene/Phenol	Phosphates

In ethanol dehydration. glycerine requires higher energy compared to ethylene glycol because of its higher boiling temperature (290°C) [33]. Thus, extractive distillation using ethylene glycol as an entrainer is conducted to break azeotrope in this work.

Ethylene glycol has a strong affinity to water. As such, when in contact with water in the ethanol/water stream, ethylene glycol will extract and bring water molecules together. Additionally, the boiling temperature of ethylene glycol (198°C) has a distinctly different from that of water (100°C). Thus, in the recovery column, ethylene glycol can be easily separated from water.

2.2.3 Previous work regarding the simulation of acetaldehyde production

For the simulation of acetaldehyde production process, there are only a few works that study involved. Johanna [34] had simulated and designed the plant for producing acetaldehyde from ethanol and ChemCAD was used for process simulation and economic evaluation. The simulation results indicated that the plant could be produced the amounts of acetaldehyde production of about 2,122 kg/h. The total capital and operating cost were 40 million SEK and 7,081 SEK/ton of acetaldehyde, respectively. A payback time on his process was 2.6 years.

The process simulation has several advantages to the design of manufacturing acetaldehyde, for instance;

- Visualize the behavior of production process without building the plant.
- Identify some risks that may occur in the process.
- Provide the effects of process variables on the process performances.
- The economic evaluator available in a process simulator can provide the profitability or viability of the process that could suggest the investment direction.

As we know, the different results such as conversion, selectivity and by-products are obtained if the different conditions are used. In this work, two processes at different operating temperature (namely 200 and 300°C) of acetaldehyde production via partial oxidative dehydrogenation of ethanol using V-Zr-La/SBA-15 as the catalysts are simulated for comparative purposes.

The noteworthy aspects of this work compared to Johanna's work is;

1) Different separation processes as a result of different conditions.

   Acetaldehyde production over V-Zr-La/SBA-15 catalyst at reaction temperature of 200 and 300°C provide 11% and 98% conversion of ethanol, respectively. This leads to a different separation scheme contributed to different investment costs. This will be beneficial to prospective producers in making their investment decisions.

2) Effect of DEE by-product on acetaldehyde purity.

All of catalysts have their own benefits. From the literature reported by Johanna [34], by-products including acetic acid, CO, CO_2, CH_4 and water are produced in acetaldehyde production using Ag catalyst. There are no by-products that directly affect the acetaldehyde purity particularly the DEE that forms azeotrope with acetaldehyde. This work will provide a useful insight whether the small amount of DEE could affect the purity of the obtained acetaldehyde. If it does affect, to what extent would it affect the separation cost. Thus, we can recommend to the catalysis research group for improvement of catalyst performance in ethanol oxidative dehydrogenation.

3) Evaluation of CO_2 emissions

The amount of CO_2 produced from the process is one of the important factors affecting the process performance since the CO_2 concentrations emitted into the atmosphere are directly related to the energy consumption and environmental impact. With regard to Johanna's process [34], the CO_2 emissions were not evaluated. Accordingly, this work will provide such important impact.

2.2.4 Enhancement of energy efficiency

One of the factors affecting the profitability is energy used in the process, which is directly related to the operating cost – the higher energy consumption the higher operating cost. Therefore, the maximum energy recovery for systems is necessary, which can be managed using the heat exchanger network (HEN). Several authors have performed the design of HEN in their process and the results are represented according to the list below (see Table 8).

Table 8. The amount of heat recovery with and without HEN

Process	Before recovery		After recover		Ref.
	Heat load (kW)	Cooling load (kW)	Heat load (kW)	Cooling load (kW)	
VCM (vinyl chloride monomer) distillation unit	254.99	256.53	215.78	134.67	[35]
Biochemical ethanol production from straw	113,000	100,000	61,000	49,000	[36]
Biomass steam gasification for hydrogen production	0.6009	0.4514	0.1642	0.0545	[37]
Cumene production from benzene and propylene	9,143.40	11,063.90	5,330	8,005	[38]

Notice that energy saving can be achieved with heat recovery system as depicted in the given table. In the process, there are more than one heat exchanger used. Accordingly, heat recovery should be performed in our work.

CHAPTER III
METHODOLOGY

This chapter describes in detail the research methodology for simulation and techno-economic analysis of acetaldehyde production from ethanol. It is divided into 6 main parts including simulation data, feedstock estimation, preliminary design, process description, thermodynamic model selection, and evaluations of process performance such as economic analysis, energy efficiency and CO_2 emission assessment.

3.1 Simulation data

In this work, two sets of input data based on the literatures are used to simulate the production process of acetaldehyde via vapor-phase oxidation of ethanol. The details regarding input data such as the value of the process parameters and reactor conditions are represented in Table 9. According to the information provided in the table below, one is the low conversion and the high selectivity while another one is the high conversion and the low selectivity, the case study for comparative purposes (e.g., process profitability, energy requirement, and CO_2 emissions).

Table 9. Summary of operating conditions, conversion and selectivity required for process simulation

Process	**1**	**2**
Catalyst	V-Zr-La/SBA-15	
Temperature (°C)	200	300
Pressure (atm)	1	1
Ethanol conversion (%)	11	98
Acetaldehyde selectivity (%)	99	41

3.2 Feedstock estimation

The feedstocks used for the production of acetaldehyde are ethanol and oxygen, the substrates involved in a chemical reaction.

For ethanol, a 99.5 wt% grade ethanol is purchased from the external source. For oxygen, this gas is used as an oxidant in oxidative dehydrogenation reaction that has the air consisting of approximately 20.95 mol% oxygen, 78.08 mol% nitrogen, 0.93 mol% argon, and 0.04 mol% CO_2 as an unlimited supply of oxygen in this work.

Further, in order to determine the total amount of ethanol and air that must feed into the system, Saudi Formaldehyde Chemical Company with an acetaldehyde production capacity of 12,000 tons/year and Eastman Chemical Company with an acetaldehyde production capacity of 120,000 tons/year are fixed and used to determine the size of a process at the reactor outlet stream, which can be made this process economically feasible [39, 40]. Additionally, other three assumed capacities (30,000, 60,000, and 90,000 tons/year) will also be determined to see the trend of each capacity on process performance.

From stoichiometric ratio, if the partial oxidation of 1 mole of ethanol is utilized, 1 mole of acetaldehyde is then generated. Table 10 shows the calculated results of 99.5 wt% ethanol and air used to produce acetaldehyde, which is the amount entering the reactor. The calculation procedures for determining the amount of these two reactants are provided in Appendix A.

Table 10. The raw material quantities need for acetaldehyde production

Temperature (°C)	**200**		**300**	
Capacity (tons/year)	Mass flow rate (tons/year)		Mass flow rate (tons/year)	
	Ethanol	Air	Ethanol	Air
12,000	116,938.31	18,853.14	24,947.13	68,285.14
30,000	292,345.78	47,132.84	62,367.81	170,712.84
60,000	584,691.55	94,265.68	124,735.63	341,425.68
90,000	877,037.33	141,398.51	187,103.44	512,138.52
120,000	1,169,383.10	188,531.35	249,471.26	682,851.36

3.3 Conceptual design

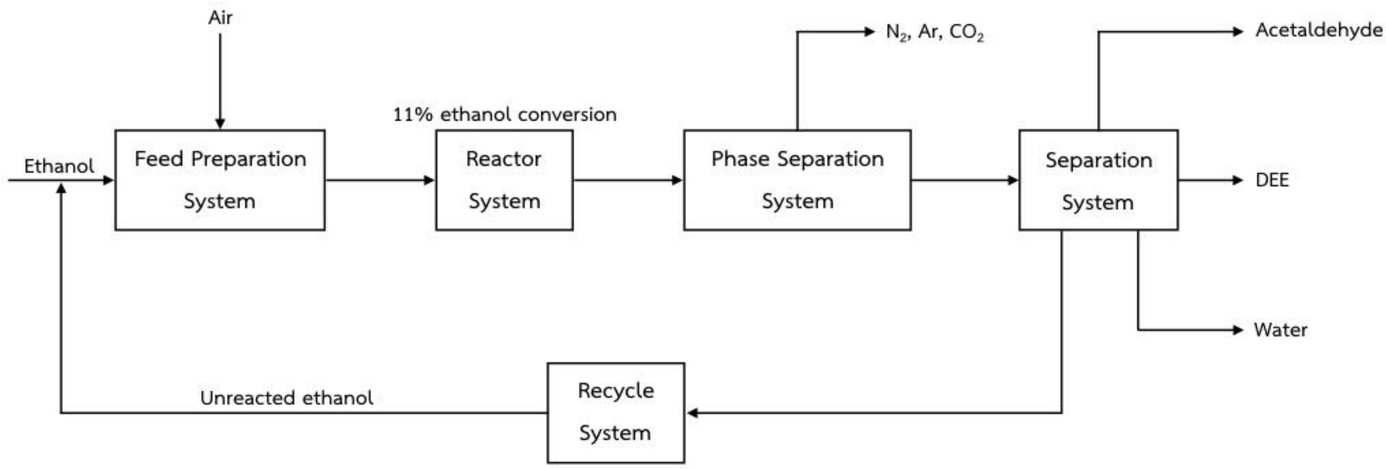


Figure 3. Block flow diagram of acetaldehyde production using V-Zr-La/SBA-15 catalyst at 200°C

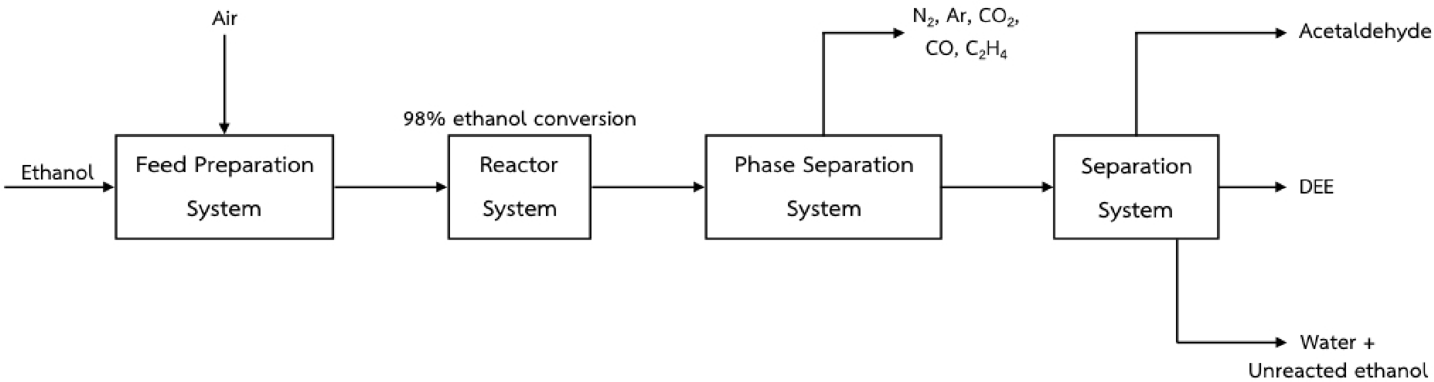


Figure 4. Block flow diagram of acetaldehyde production using V-Zr-La/SBA-15 catalyst at 300°C

The two figures above are the conceptual design to produce acetaldehyde from ethanol using different conditions, which can be divided into 5 systems including:

3.3.1 Feed preparation system

The raw materials used in both processes are stored in the storage tank at the temperature and pressure of 30°C and 1 atm. Thus, the system for preparing the conditions is necessary since the suitable conditions for acetaldehyde production via partial oxidative dehydrogenation of ethanol using V-Zr-La/SBA-15 catalyst is 200 and 300°C at constant pressure of 1 atm as seen in Table 9.

3.3.2 Reactor system

After preparing the conditions, the ethanol oxidation reactions will take place to produce the desired products in this system. Regarding the acetaldehyde production reactor system, the isothermal reactor is operated for both processes at a constant pressure of 1 atm. The WHSV is used to be calculated the size of reactor in this work.

3.3.3 Phase separation system

Upon leaving the reactor, the reactor effluents in both processes are all vapor which must be cooled down for achieving the gas-liquid phase split in a phase separator, namely flash drum. Each stream exiting the flash drum consists of components shown in Table 11.

Table 11. The components in the gas and liquid streams of both processes

Process	Catalyst	Temperature (°C)	Gas stream	Liquid stream
1	V-Zr-La/SBA-15	200	N_2, Ar, CO_2	Acetaldehyde, water, DEE and unreacted ethanol
2		300	N_2, C_2H_4, Ar, CO and CO_2	Acetaldehyde, water, DEE and unreacted ethanol

3.3.4 Separation system

The functions of this system are used to separate and purify the mixtures comprised of two or more components in order to gain the high purity products. The main type of equipment used in separation system is the distillation column. The design of the distillation columns is conducted by means of “DSTWU” short-cut model in Aspen Plus, to establish four significant variables - that is the reflux ratio (RR), number of stages, feed location, and distillate rate (kmol/h). After that, the rigorous model “RADFRAC” is used for adjusting the RR or distillate rate values with Design Spec feature so as to obtain the desired purity. In this work, acetaldehyde with a product purity of 99 wt% is required.

3.3.5 Recycle system

In partial oxidative dehydrogenation of ethanol using V-Zr-La/SBA-15 as the catalyst at reaction temperature of 200°C, the chemical reaction gives 11% conversion of ethanol. Thus, the unreacted ethanol must be recycled back to conserve materials. Whereas, in the case of 300°C, the ethanol oxidation gives 98% conversion of ethanol. As a result, ethanol recycling system is not necessary at all.

3.4 Process description

By using Aspen Plus Process Simulator, the process flow diagrams of acetaldehyde production processes are depicted in Figure 6 and Figure 7 for the operating temperature of 200 and 300°C, respectively.

3.4.1 Partial oxidative dehydrogenation of ethanol at 200°C

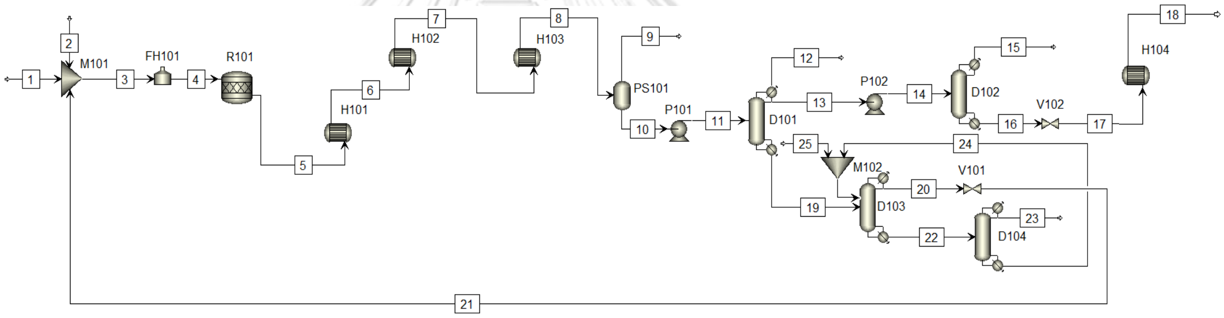


Figure 5. Process flow diagram of acetaldehyde production at 200°C

As seen in Figure 5, a 99.5 wt% fresh feed of ethanol (stream 1^{st}), the air stream 2^{nd}, and ethanol recycle stream 21^{th} are mixed in the mixer, M101. Then, the mixed stream 3^{rd} is delivered to a fired heater, FH101. This equipment increases the temperature of the ethanol-air mixture (stream 3^{rd}) to 200°C, the desired temperature for acetaldehyde production. The stream 4^{th} exiting the FH101 is then fed to a reactor, R101 for carrying out the ethanol partial oxidative reaction. After the reaction, the stream 5^{th} is sent to a series of the shell and tube heat exchangers, H101, H102 and H103. First, the hot stream 5^{th} is cooled from the temperature of 200 to about 121°C before entering the secondary heat exchanger, H102 where the stream temperature is decreased further to 45°C. Next, the temperature of stream 7^{th}

is decreased to 10°C in H103 and then sent to a flash drum, PS101 to separate the cooled stream 8th into two distinct phases, namely gas and liquid phase. The liquid stream from PS101 that consists mainly of ethanol, water, acetaldehyde and a small amount of DEE is sent to a pump, P101 where the stream pressure is raised from 1 to 2.34 bar before entering the distillation column, D101. This column has divided into three streams including 1) the gas stream 12th that composes of the remaining gas, 2) the liquid stream 13th that contains an acetaldehyde-DEE azeotropic mixture, and 3) the liquid streams 19th that is fed into the distillation column, D103 and D104 for unreacted ethanol and ethylene glycol recovery, respectively. An acetaldehyde-DEE azeotrope in stream 13th is sent to a pump, P102 which has a discharge pressure of 2.54 bar. The stream 14th from P102 is fed into the distillation column, D102 where the acetaldehyde with a purity of 99 wt% is achieved. Finally, the product stream 16th at 2.54 bar and 47.20°C is sent to a valve V102 and a heat exchanger H104, respectively, for reducing the stream pressure to 2.05 bar and the stream temperature to 30°C, the storage condition for the obtained product.

3.4.2 Partial oxidative dehydrogenation of ethanol at 300°C

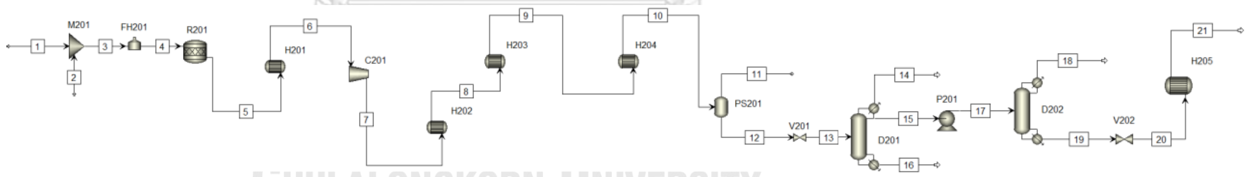


Figure 6. Process flow diagram of acetaldehyde production at 300°C

In accordance with the figure, a solution of 99.5 wt% ethanol (stream 1st) is mixed with the air stream 2nd in a mixer, M201 before entering the fired heater, FH201 that raises the mixed stream temperature to 300°C, the operating condition of producing acetaldehyde from ethanol. Then, the stream 4th is fed into a reactor, R201. In the reactor, partial oxidative dehydrogenation of ethanol takes place and gives acetaldehyde as the major product as well as five chemical by-products including CO_2, CO, ethylene, DEE and water. Upon leaving the reactor, the product stream 5th is sent to the shell and tube heat exchanger, H201 where the stream 6th with the temperature of 90°C is obtained. The discharge from H201 is delivered to a compressor, C201 to increase the stream pressure from 1 to 10 bar. After C201, the stream 7th is passed through the shell and tube heat exchangers as follows, H202, H203 and H204. These three heat exchangers are used to cool down the temperature of stream 7th from about 429 to 10°C. Next, the cooled product in stream 10th is fed into a gas-liquid phase separator, PS201. The liquid stream 12th from PS201 at a pressure of 10 bar is sent to a valve, V201 and then exited the V201 at 2.34 bar. Further, the stream 13th is fed into the distillation column, D201 where three streams are acquired, two at the top and one at the bottom. The distillate stream 15th from D201 is sent to a pump, P201 for increasing the stream pressure to 2.84 bar before entering the distillation column, D202 that separates and purifies the inlet stream 17th to obtain 99 wt% acetaldehyde appeared in stream 19th. Lastly, to store the finished product securely, the product stream 21th at 2.05 bar and 30°C is achieved by using a valve V202 and a heat exchanger H205, respectively.

3.5 Thermodynamic model used in this study

As seen in Table 9, the operating conditions of these two processes for acetaldehyde synthesis are carried out at low pressure. Also, both processes consist of polar molecules and binary azeotropes (i.e., ethanol-water and DEE-acetaldehyde mixture). Therefore, according to Eric Carlson's guideline [41], the activity coefficient model (NRTL) is selected to describe the acetaldehyde production processes.

3.6 Evaluations of process performance

3.6.1 Raw material utilization

The raw material utilization is used to describe the efficiency of converting raw materials into desirable products. In this work, the important raw materials and valuable products are ethanol and acetaldehyde, respectively. If the quantitative conversion of ethanol into acetaldehyde in the process is high, the process will be efficient in using raw materials.

3.6.2 Economic analysis

In this work, the techno-economic aspects of acetaldehyde production process can be evaluated by the Economic Evaluator in Aspen Plus. The ethanol and acetaldehyde cost are estimated to be about 0.49 $/L and 1.01 $/kg, respectively [42, 43]. A list of utility prices is provided in Table 12 [44].

Table 12. Summary of utility prices

Utility	Price	Unit
Electricity	0.06	US$/kWh
Cooling water	0.067	US$/ton
Chilled water	0.185	US$/ton
Boiler feed water	2.45	US$/ton
Low pressure steam	12.68	US$/ton
Medium pressure steam	13.71	US$/ton
High pressure steam	16.64	US$/ton
Natural gas	6.0	US$/GJ

The index that quantify the economic performance of the process is Profitability Index (PI) which can be calculated by the following equation.

$$\textbf{Profitability Index (PI)} = \frac{\textbf{Present Value of Future Cash Flows}}{\textbf{Initial Investment}} \tag{3.1}$$

The rules of Profitability Index are that:

- If PI is greater than 1, the project should be accepted.
- If PI is less than 1, the project should be rejected.

As mentioned above, the PI value only indicates the viability of the project, but unable to determine the time period of returning the capital investment and profit rate. Therefore, there must be other parameters to answer these issues including 1) Internal Rate of Return (IRR) - a financial indicator used to measure and evaluate the profitability of the project, and 2) Pay-out Period (POP) - how many years will the project return the total investment costs. These three parameters can be determined by the software in Aspen Plus.

3.6.3 Energy efficiency

Energy efficiency is a significant factor to consider the process performance and economic outcomes. In this work, it is referred as specific energy consumption (SEC) which is calculated in accordance with Eq. (3.2) [45].

$$\text{SEC} = \frac{\text{Energy used}}{\text{Product's amount}} \tag{3.2}$$

In the present work, thermal and electrical duties are measured as the term of energy used and then divided by the total amount of acetaldehyde produced.

For the improvement of energy efficiency, it can be handled with heat exchanger network (HEN) to recover the energy of processes.

3.6.4 CO_2 emission assessment

Due to the effect of CO_2 on global climate change, the total amounts of CO_2 released from the two acetaldehyde production processes are also considered. Two possible sources of emitting CO_2 in this work include the utility usage and chemical reaction which are indirect and direct CO_2 emissions, respectively. The net CO_2 emission can be computed from Eq. (3.3).

$$\text{Net CO}_2\text{ emission} = \sum_{n}^{i} CO_{2\,outlet} - \sum_{n}^{i} CO_{2\,inlet} \tag{3.3}$$

CHAPTER IV
RESULTS AND DISCUSSION

The obtained results of this study are explained and interpreted in this chapter, which can be divided into 7 major sections including raw material utilization, the simulated results of acetaldehyde production, economic analysis, energy efficiency, CO_2 emission assessment, heat recovery, and recommendation for future work.

4.1 Raw material utilization

The total ethanol feed rates for producing acetaldehyde at 200 °C and 300 °C are provided in Table 13. In partial oxidative dehydrogenation of ethanol at 200°C, about 11% conversion of ethanol (a single-pass conversion) is achieved in the reactor. As such, two ethanol streams including fresh feed and recycle streams are presented in this acetaldehyde production process. For the process operated at 300 °C, because of high ethanol conversion (98%), there is no need to recover the ethanol. Thus, this process has 98% overall conversion of ethanol.

As seen in the table, these estimated values are calculated from the stoichiometric coefficients in the balanced chemical equations based on the assumption of perfect separations. This means that the amount of ethanol is not lost (e.g. in distillation columns involved in ethanol recovery) during the production process.

Table 13. The amount of 99.5 wt% ethanol obtained by the stoichiometric calculation

T (°C)	Ethanol flow rate (tons/year)	Stream No.	Acetaldehyde production capacity (tons/year)				
			12,000	**30,000**	**60,000**	**90,000**	**120,000**
200	Fresh feed	1	12,863.21	32,158.04	64,316.07	96,474.11	128,632.14
	Recycle	21	104,075.10	260,187.74	520,375.48	780,563.22	1,040,750.96
300	Fresh feed	1	24,947.13	62,367.81	124,735.63	187,103.44	249,471.26
	Recycle	-	-	-	-	-	-

However, the perfect separation will never be attained. Table 14 summarizes the results of ethanol quantities in stream number 1st and 21th after finishing the simulation of acetaldehyde production process at temperature of 200 °C. According to the table, the simulated results show that the amount of ethanol in both streams is not equal to the values appeared in Table 13.

Table 14. The amount of 99.5 wt% ethanol obtained by the process simulation of acetaldehyde production at 200 °C

Ethanol flow rate (tons/year)	Stream No.	Acetaldehyde production capacity (tons/year)				
		12,000	**30,000**	**60,000**	**90,000**	**120,000**
Fresh feed	1	13,988.81	34,971.37	69,944.51	104,912.79	139,885.48
Recycle	21	102,950.33	257,374.55	514,746.49	772,124.08	1,029,497.86

Since some ethanol has lost during the separation and purification process, the amount of ethanol in the recycle stream is less than the calculated values in Table 13. As a result, the lost ethanol is compensated by adding the ethanol to the fresh feed stream. The compensation percentages are about 8% in all cases (Take the 12,863 tons/year VS 13,988 tons/year for example, which is about 8% compensation in 12,000 tons/year acetaldehyde production case). Since the process operated at 200°C has water as a by-product, the azeotrope formed between ethanol and water makes the separation more difficult as seen by the 8% compensation of ethanol. In other words, about 92% of the overall conversion of ethanol is achieved when the process in Figure 5 is applied.

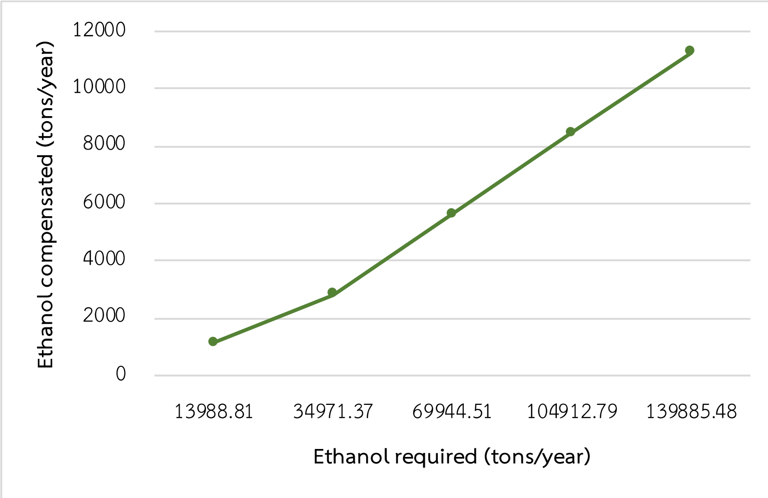


Figure 7. The relationship between ethanol requirement and ethanol compensation for acetaldehyde production at 200°C

To confirm that the obtained material balance is correct, Figure 7 presents the correlation of the ethanol quantities required for acetaldehyde production and the compensated amount of ethanol. Because of the mass balance constraint, the compensation of ethanol increases linearly with the required amounts of ethanol.

By comparing the results from the operating temperatures at 200 °C and 300 °C, it appears that the 300 °C case yields better utilization of raw material as the overall conversion of ethanol is closer to 100%. However, if considered ONLY the portion of ethanol converted to acetaldehyde, the process performed at temperature of 300°C has a lower efficiency in using raw materials than that of 200°C as appeared in Figure 8. Also note that the “Total” in Figure 8 stands for the total amount of ethanol in the fresh feed stream whereas the “ACT” stands for the portion of ethanol in the fresh feed that is converted into acetaldehyde.

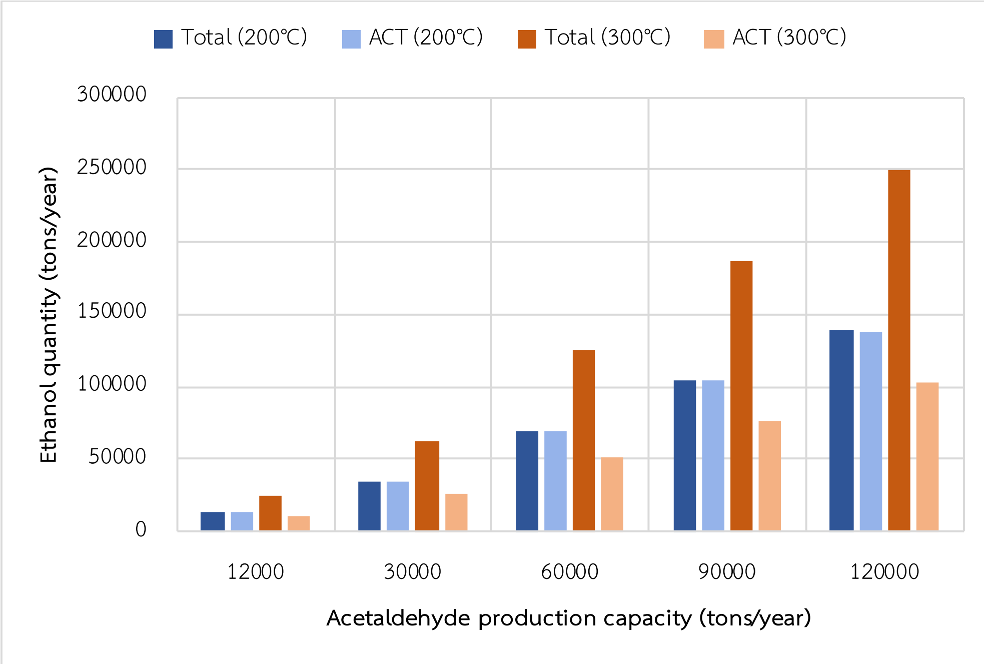


Figure 8. The total amount of ethanol used in the process compared to the amount of ethanol used in producing acetaldehyde

From the figure, the quantitative conversion of ethanol to produce acetaldehyde in the case of operating at 300°C is lower - although partial oxidative dehydrogenation of ethanol at 300°C gives a high conversion of ethanol (98%), the selectivity of acetaldehyde is only 41%. In contrast to 200°C case, just 11% conversion of ethanol takes place in the reactor but the chemical reaction provides 99% selectivity of acetaldehyde. Therefore, acetaldehyde production at 200°C is better than the production at 300°C since the majority of ethanol is converted into acetaldehyde.

4.2 The simulated results of acetaldehyde production by Aspen Plus

According to the process flow diagrams presented in Chapter 3, Section 3.4, stream results of acetaldehyde production under different operating conditions are represented in Table 15-16. However, this only shows the results of the manufacturing process having an acetaldehyde production capacity of 120,000 tons/year. For other capacities, stream results are provided in Appendix C.

Table 15. Stream results of acetaldehyde production at 200℃

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	℃	30	30	52.49	200	200	120.89	45
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Molar Vapor Fraction		0	1	0.3023	1	1	1	0.2262
Mole Flows	kmol/hr	316.684	673.585	3319.57	3319.57	3460.45	3460.45	3460.45
Mass Flows	tons/year	139885	188531	1.3579E+06	1.3579E+06	1.3579E+06	1.3579E+06	1.3579E+06
Ethanol	tons/year	139186	0	1.1635E+06	1.1635E+06	1.0356E+06	1.0356E+06	1.0356E+06
Oxygen	tons/year	0	43633.1	43633.1	43633.1	72.5378	72.5378	72.5378
Nitrogen	tons/year	0	142366	142366	142366	142366	142366	142366
Argon	tons/year	0	2418.11	2418.11	2418.11	2418.11	2418.11	2418.11
Carbon dioxide	tons/year	0	114.58	114.58	114.58	114.58	114.58	114.58
Acetaldehyde	tons/year	0	0	306.434	306.434	120247	120247	120247
Diethyl ether	tons/year	0	0	5.8640	5.8640	2065.14	2065.14	2065.14
Water	tons/year	699.427	0	5461.86	5461.86	55011.4	55011.4	55011.4
Ethylene glycol	tons/year	0	0	72.7977	72.7977	72.7977	72.7977	72.7977

Table 15. Stream results of acetaldehyde production at 200°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	10	10	10	10.08	31.06	31.06	31.11
Pressure	bar	1.01325	1.01325	1.01325	2.34	2	2	2.54
Molar Vapor Fraction		0.1607	1	0	0	1	0	0
Mole Flows	kmol/hr	3460.45	556.22	2904.23	2904.23	2.7844	275.656	275.656
Mass Flows	tons/year	1.3579E+06	155031	1.2029E+06	1.2029E+06	1082.27	117556	117556
Ethanol	tons/year	1.0356E+06	5946.68	1.0296E+06	1.0296E+06	0.0286	102.921	102.921
Oxygen	tons/year	72.5378	72.3558	0.1821	0.1821	0.1584	0.0236	0.0236
Nitrogen	tons/year	142366	142157	208.85	208.85	191.179	17.671	17.671
Argon	tons/year	2418.11	2411.68	6.4306	6.4306	6.3726	0.0580	0.0580
Carbon dioxide	tons/year	114.58	110.275	4.3046	4.3046	3.6612	0.6434	0.6434
Acetaldehyde	tons/year	120247	3690.63	116557	116557	859.273	115391	115391
Diethyl ether	tons/year	2065.14	323.658	1741.49	1741.49	20.7447	1714.88	1714.88
Water	tons/year	55011.4	319.421	54692	54692	0.8515	328.887	328.887
Ethylene glycol	tons/year	72.7977	1.165E-04	72.7976	72.7976	1.1506E-19	1.1978E-13	1.1978E-13

Table 15. Stream results of acetaldehyde production at 200°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	41.52	47.20	40.66	30	100.89	96.52	78.24
Pressure	bar	2.2	2.54	2.05	2.05	2.34	2	1.01325
Molar Vapor Fraction		1	0	0.0365	0	0	0	0.0714
Mole Flows	kmol/hr	12.3469	263.309	263.309	263.309	2625.79	2329.3	2329.3
Mass Flows	tons/year	5661.77	111894	111894.13	111894.13	1.0843E+06	1.0295E+06	1.0295E+06
Ethanol	tons/year	1.7984E-11	102.921	102.921	102.921	1.0295E+06	1.0244E+06	1.0244E+06
Oxygen	tons/year	0.0236	3.375E-30	3.375E-30	3.375E-30	1.13E-16	0	0
Nitrogen	tons/year	17.671	1.7499E-29	1.7499E-29	1.7499E-29	1.7607E-14	0	0
Argon	tons/year	0.0580	4.8266E-45	4.8266E-45	4.8266E-45	5.7654E-15	0	0
Carbon dioxide	tons/year	0.6434	2.8305E-30	2.8305E-30	2.8305E-30	3.8496E-11	0	0
Acetaldehyde	tons/year	4615.63	110775	110775	110775	306.434	306.434	306.434
Diethyl ether	tons/year	1027.28	687.599	687.599	687.599	5.8640	5.8640	5.8640
Water	tons/year	0.4660	328.421	328.421	328.421	54362.2	4762.43	4762.43
Ethylene glycol	tons/year	0	0	0	0	72.7976	72.7974	72.7974

Table 15. Stream results of acetaldehyde production at 200°C (Cont'd)

Stream No.	Unit	22	23	24	25	26
Temperature	°C	159.74	110.92	227.33	227.40	227.33
Pressure	bar	2.34	2	2.34	2.34	2.34
Molar Vapor Fraction		0	0	0	0	3.6608E-09
Mole Flows	kmol/hr	1006.61	296.777	709.837	0.287	710.124
Mass Flows	tons/year	480598	54919.5	425678	172.131	425850
Ethanol	tons/year	5157.59	5157.59	0.00313	0	0.00313
Oxygen	tons/year	0	0	0	0	0
Nitrogen	tons/year	0	0	0	0	0
Argon	tons/year	0	0	0	0	0
Carbon dioxide	tons/year	0	0	0	0	0
Acetaldehyde	tons/year	7.725E-05	7.725E-05	3.455E-11	0	3.4555E-11
Diethyl ether	tons/year	2.468E-06	2.468E-06	9.457E-12	0	9.4879E-12
Water	tons/year	49621.3	49599.8	21.5224	0	21.5229
Ethylene glycol	tons/year	425829	172.128	425657	172.131	425829

Table 16. Stream results of acetaldehyde production at 300℃

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	℃	30	30	8.17	300	300	90	429.05
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	10
Molar Vapor Fraction		0	1	0.8350	1	1	1	1
Mole Flows	kmol/hr	564.773	2439.69	3004.47	3004.47	3470.12	3470.12	3470.12
Mass Flows	tons/year	249471	682851	932323	932323	932323	932323	932323
Ethanol	tons/year	248224	0	248224	248224	4964.48	4964.48	4964.48
Oxygen	tons/year	0	158037	158037	158037	245.189	245.189	245.189
Nitrogen	tons/year	0	515641	515641	515641	515641	515641	515641
Argon	tons/year	0	8758.28	8758.28	8758.28	8758.28	8758.28	8758.28
Carbon dioxide	tons/year	0	415.002	415.002	415.002	63254.1	63254.1	63254.1
Acetaldehyde	tons/year	0	0	0	0	119963	119963	119963
Carbon monoxide	tons/year	0	0	0	0	39994.4	39994.4	39994.4
Ethylene	tons/year	0	0	0	0	27948.8	27948.8	27948.8
Diethyl ether	tons/year	0	0	0	0	4932.34	4932.34	4932.34
Water	tons/year	1247.36	0	1247.36	1247.36	146621	146621	146621

Table 16. Stream results of acetaldehyde production at 300°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	139.40	45	10	10	10	9.96	34.48
Pressure	bar	10	10	10	10	10	2.34	2
Molar Vapor Fraction		1	0.7426	0.6928	1	0	3.1346E-04	1
Mole Flows	kmol/hr	3470.12	3470.12	3470.12	2404.02	1066.1	1066.1	6.48375
Mass Flows	tons/year	932323	932323	932323	688993	243330	243330	2738.8
Ethanol	tons/year	4964.48	4964.48	4964.48	43.155	4921.32	4921.32	1.9165E-05
Oxygen	tons/year	245.189	245.189	245.189	245.143	0.0463	0.0463	0.0440
Nitrogen	tons/year	515641	515641	515641	515593	48.545	48.545	46.9823
Argon	tons/year	8758.28	8758.28	8758.28	8756.52	1.7593	1.7593	1.7568
Carbon dioxide	tons/year	63254.1	63254.1	63254.1	62900.6	353.475	353.475	342.413
Acetaldehyde	tons/year	119963	119963	119963	29748.4	90214.4	90214.4	2256.49
Carbon monoxide	tons/year	39994.4	39994.4	39994.4	39988.9	5.56865	5.56865	5.3299
Ethylene	tons/year	27948.8	27948.8	27948.8	27927.9	20.8552	20.8552	20.7557
Diethyl ether	tons/year	4932.34	4932.34	4932.34	3362.4	1569.94	1569.94	62.1882
Water	tons/year	146621	146621	146621	427.129	146194	146194	2.8379

Table 16. Stream results of acetaldehyde production at 300°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	34.48	119.40	34.56	45.44	50.70	40.63	30
Pressure	bar	2	2.34	2.84	2.5	2.84	2.05	2.05
Molar Vapor Fraction		0	0	0	1	0	0.0564	0
Mole Flows	kmol/hr	209.641	849.978	209.641	9.5636	200.078	200.078	200.078
Mass Flows	tons/year	89471.4	151120	89471.4	4440.26	85031.19	85031.19	85031.19
Ethanol	tons/year	0.0176	4921.31	0.0176	6.996E-15	0.0176	0.0176	0.0176
Oxygen	tons/year	0.0023	2.2793E-18	0.0023	0.0023	4.0065E-40	4.0065E-40	4.0065E-40
Nitrogen	tons/year	1.5627	1.5924E-16	1.5627	1.5627	3.5413E-40	3.5413E-40	3.5413E-40
Argon	tons/year	0.0026	1.0207E-16	0.0026	0.0026	1.00E-64	1.00E-64	1.00E-64
Carbon dioxide	tons/year	11.0627	3.337E-09	11.0627	11.0627	8.3447E-42	8.3447E-42	8.3447E-42
Acetaldehyde	tons/year	87688.4	269.51	87688.4	3507.54	84180.9	84180.9	84180.9
Carbon monoxide	tons/year	0.2387	8.5706E-17	0.2387	0.2387	3.0664E-39	3.0664E-39	3.0664E-39
Ethylene	tons/year	0.0995	2.86E-13	0.0995	0.0995	9.0445E-56	9.0445E-56	9.0445E-56
Diethyl ether	tons/year	1507.75	0.0027	1507.75	918.235	589.513	589.513	589.513
Water	tons/year	262.298	145929	262.298	1.5167	260.781	260.781	260.781

4.3 Economic analysis

In this work, the techno-economic analysis of acetaldehyde production processes is conducted by Aspen Economic Analyzer with a fixed 20 years project lifetime. The production capacity of acetaldehyde set up for economic evaluation has been divided into five capacities including two based cases (12,000 and 120,000 tons/year) and other three assumed cases (30,000, 60,000, and 90,000 tons/year). From Independent Commodity Intelligence Services (ICIS) pricing data, ICIS has the acetaldehyde selling price of about $1.01 per kilogram, which is the reference price for acetaldehyde used in this work [43]. However, according to the reference price, the economic results of each acetaldehyde production size indicate that the processes (both 200 and 300°C) cannot make a profit during 20 years of the project lifetime. Therefore, finding the new price of acetaldehyde to improve profitability of production processes is essential. Please note that 0.49 $ per liter is fixed and used as the price of ethanol for techno-economic evaluation [42].

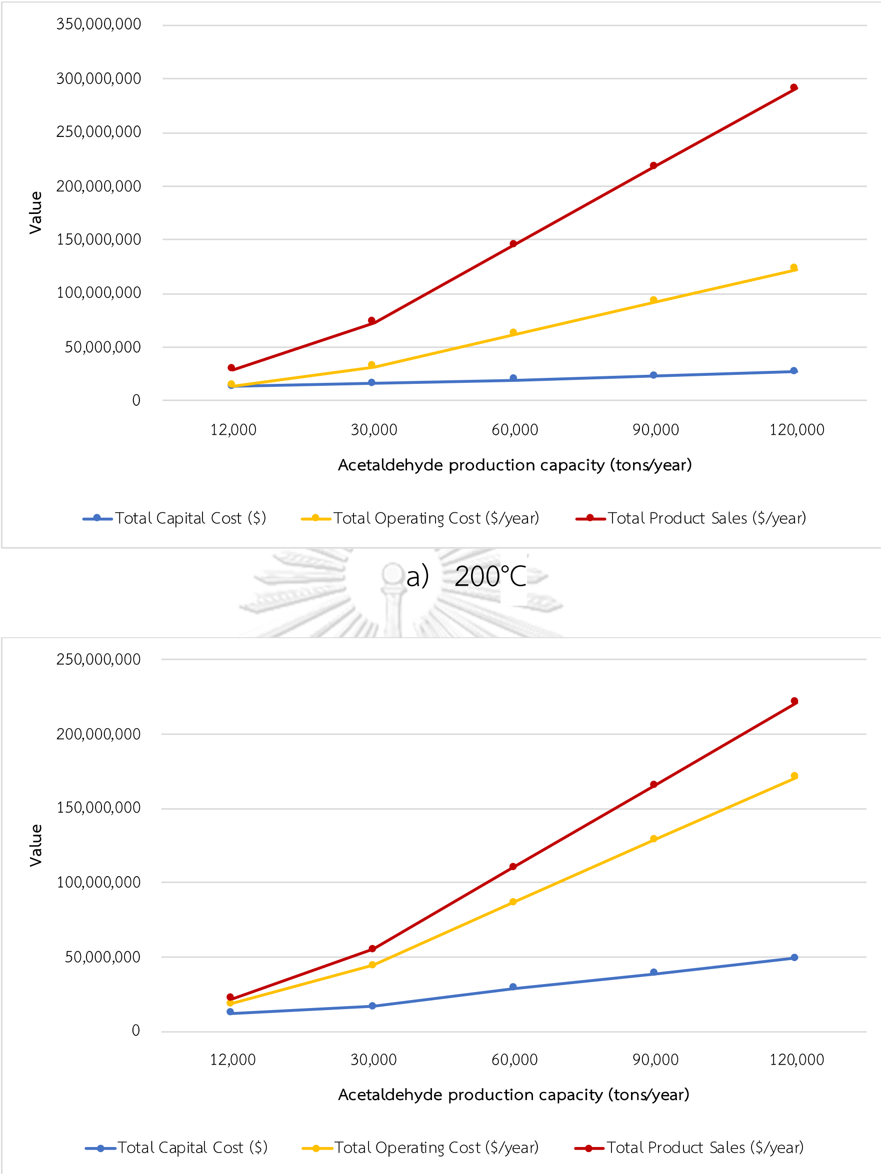
Among five capacities mentioned above, the ethanol oxidation process having a capacity of 120,000 tons of acetaldehyde per year is chosen to determine the minimum acetaldehyde selling price that begins to turn a profit in this work. Since the process is expected to be more profitable if higher production capacity is used, the maximum production capacity is selected as the first choice for economic evaluation. In addition, at this capacity, the acetaldehyde price is determined based on the 5 years of payout period (POP). This price is then utilized for evaluating the economic efficiency of acetaldehyde production processes to decide the suitable condition with the optimal production capacity for acetaldehyde synthesis that uses ethanol as a starting material.

By using the Economic Evaluator in Aspen Plus, for partial oxidative dehydrogenation of ethanol with a production capacity of 120,000 tons per year of acetaldehyde, the starting price of acetaldehyde that has a potential of returning profit at year 20th is equal to 1.33 and 2.50 $/kg for 200 and 300°C, respectively. Regarding the price of acetaldehyde that leads to a POP of about 5 years, it is approximately 1.52 $/kg for 200°C and 2.86 $/kg for 300°C. Thus, the selected price used for determining the optimal production capacity is assumed at 2.86 $/kg. Results of the economic evaluation are summarized in Table 17.

Table 17. Profitability Index (PI), Payout period (POP), and %IRR at different production capacities of acetaldehyde

T (°C)	Economic parameter	Acetaldehyde production capacity (tons/year)				
		12,000	**30,000**	**60,000**	**90,000**	**120,000**
200	PI	1.31	1.42	1.45	1.466	1.473
	POP (year)	2.86	2.02	1.83	1.774	1.77
	%IRR	73.50	124.08	150.92	161.16	166.26
300	PI	0.98	1.05	1.07	1.079	1.084
	POP (year)	-	6.36	5.52	5.14	4.95
	%IRR	-	31.51	36.20	38.81	40.29

As appeared in the table, the economic feasibility of acetaldehyde production process at 300°C with a capacity of less than 120,000 tons/year is impossible to attain with a targeted POP of no more than 5 years when the acetaldehyde price of 2.86 $/kg is assumed, except that the price of acetaldehyde will be higher. For the operating condition at 200 °C, all five cases of production capacities are acceptable because these capacities have PI greater than 1 and a POP within a few years. Therefore, ethanol transformation towards acetaldehyde at 200°C in each capacity are economically feasible given that the acetaldehyde price is 2.86 $/kg.



b) 300°C

Figure 9. Total capital cost, total operating cost, and total product sales for each acetaldehyde production process

According to Figure 9, the rate of increase of the total product sales in both conditions dominate other costs, e.g. total capital cost, and total operating cost. These results are consistent with the results in Table 17 that the higher production capacity of acetaldehyde should lead to a process with higher profit.

In addition, from the economic analysis result, the highest internal rate of return (IRR) is achieved by the maximum production capacity that uses in this work.

Therefore, the optimum capacity proposed for both acetaldehyde production processes is 120,000 tons/year.

Further, regarding the optimum operating condition for acetaldehyde synthesis, this is judged only on the profitability of the process. Another point such as the amounts of CO_2 emission are not included. In accordance with Table 17, the recommended operating temperature to produce acetaldehyde via partial oxidative dehydrogenation of ethanol using V-Zr-La/SBA-15 catalyst is 200°C because such condition provides a higher %IRR and a shorter POP when compared to another condition (i.e., 300°C).

As mentioned above, at the same price of acetaldehyde, vapor-phase ethanol oxidation at temperature of 200°C offers better profit potential than that of 300°C. This may be caused by several reasons including:

1) At 200°C, the total cost of raw materials is lower.

Table 18. Ethanol quantity required for acetaldehyde synthesis

T (°C)	Mass flow rate (tons/year) in Stream No.	Acetaldehyde production capacity (tons/year)				
		12,000	30,000	60,000	90,000	120,000
200	1	13,988.81	34,971.37	69,944.51	104,912.79	139,885.48
300	1	24,947.13	62,367.81	124,735.63	187,103.44	249,471.26

In partial oxidation of ethanol, the values of ethanol conversions observed are 11% and 98% for the operating temperature of 200 and 300°C, respectively. The higher single-pass conversion of ethanol results in the higher consumption of ethanol. Table 18 represents the total amount of 99.5 wt% ethanol consumed in the acetaldehyde production processes. From the table, it has been found that the process with a reaction temperature of 300°C uses ethanol in large quantities which is almost 1.8 times more than that of 200°C. As a result, at temperature of 300°C, the cost of raw materials purchased for producing acetaldehyde is higher when compared to another process. This can be confirmed by the economic analysis results expressed in Figure 10.

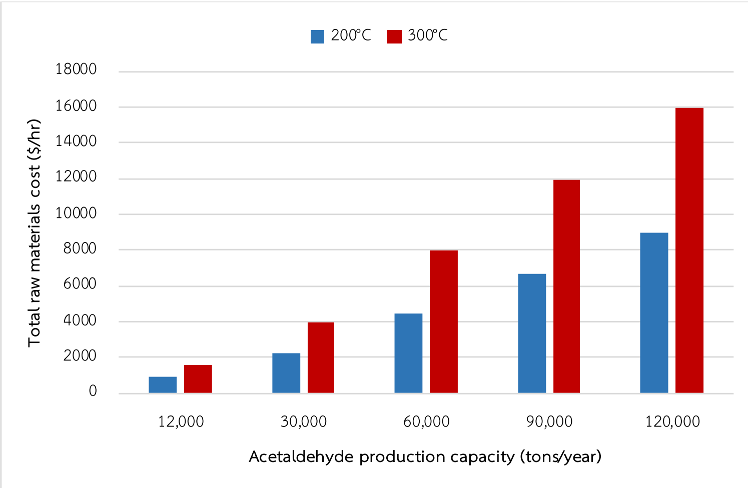
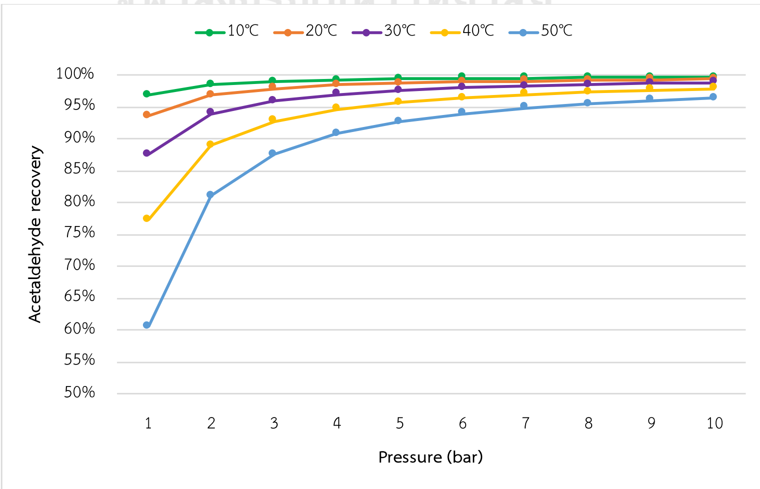


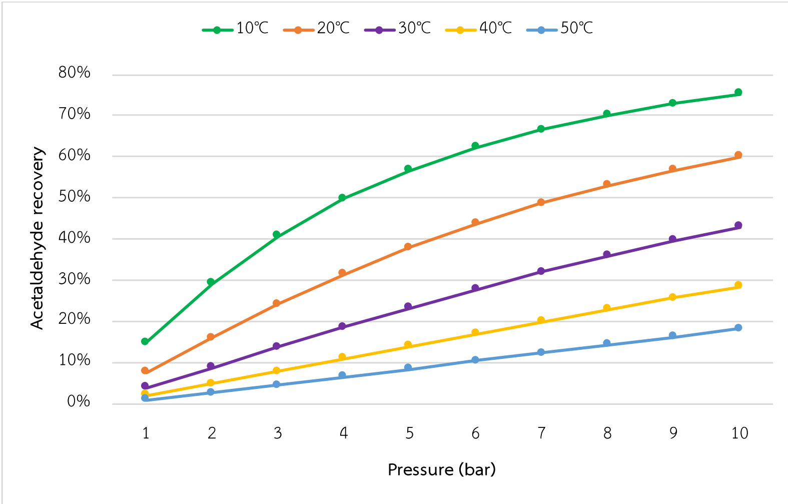
Figure 10. Results of total raw materials cost obtained by Aspen Process Economic Analyzer

2) At 300°C, the process yields a smaller amount of acetaldehyde.

By utilizing the sensitivity function in Aspen Plus (See Figure 11), the condition selected for a flash drum is at 10°C and 1 atm for the process operating at 200°C, and at 10°C and 10 bar for the process operating at 300°C which are the best condition to achieve the highest acetaldehyde recovery.



a) 200°C



b) 300°C

Figure 11. Effect of different temperatures and pressures on the amount of acetaldehyde exiting the flash drum

At 200°C, since about 97% of total acetaldehyde production is recovered after leaving the flash drum (this process produces only two by-products e.g. DEE and water) and the gas compressor is also very expensive, a flash drum with a pressure of 1 atm that does not require the installation of a compressor is sufficient.

Table 19. Acetaldehyde quantities for 200 and 300°C

T (°C)	Mass flow rate (tons/year) in Stream No. (Acetaldehyde recovery)	Acetaldehyde production capacity (tons/year)				
		12,000	30,000	60,000	90,000	120,000
200	18	11,189.49	27,973.54	55,947.00	83,920.53	111,894.13
300	21	8,503.12	21,257.79	42,515.59	63,773.39	85,031.19

In the case of 300°C, there are 5 by-products produced in the reactor (DEE, ethylene, CO, CO_2, and water). As such, some amount of acetaldehyde is lost after in a flash drum due to the gas-liquid equilibrium. Consequently, partial oxidative dehydrogenation of ethanol at the temperature of 300°C has lower acetaldehyde quantity than that of 200°C as seen in Table 19. The following table represents the total amount of 99 wt% acetaldehyde obtained from Aspen Plus. According to the table, this results in lower total product sales for 300°C, which is proven by Figure 12.

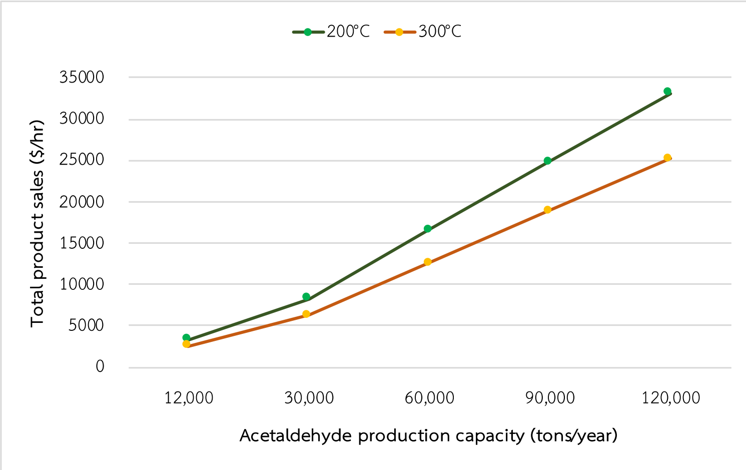


Figure 12. Results of total product sales obtained by Aspen Process Economic Analyzer

3) At 300°C, the cost of process equipment is higher.

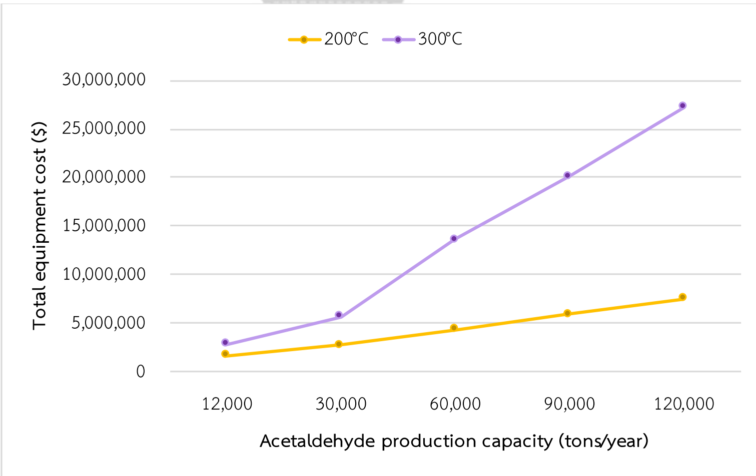
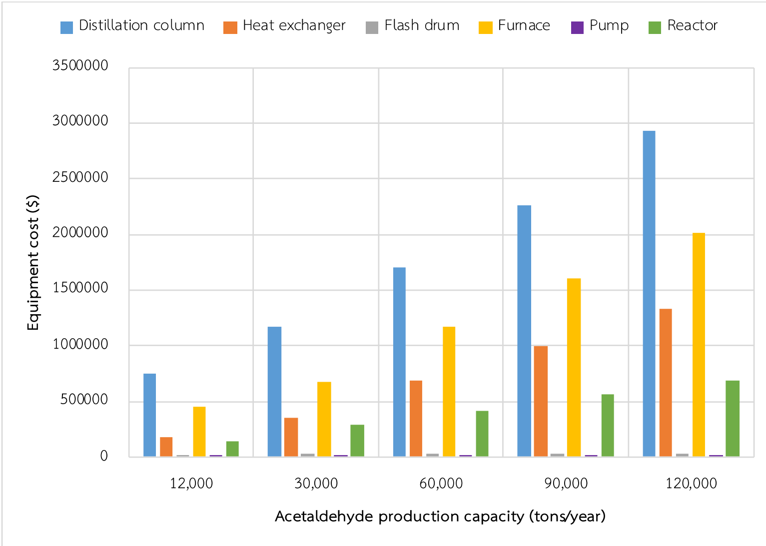
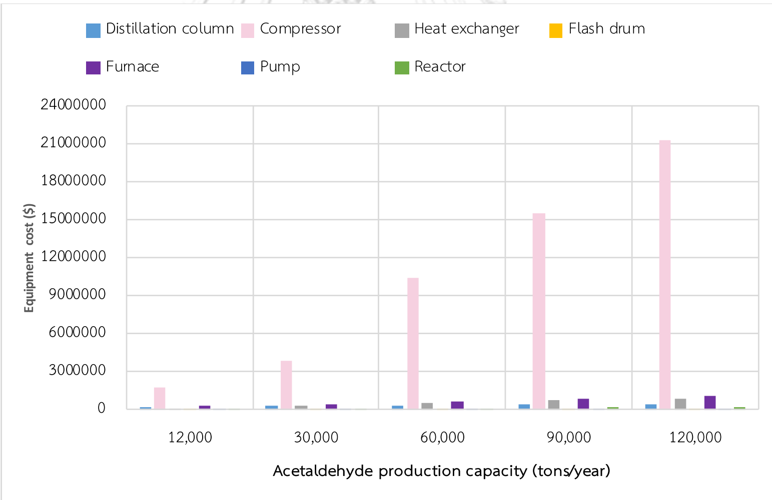


Figure 13. Results of total equipment cost obtained by Aspen Process Economic Analyzer

Total equipment costs used for acetaldehyde production at 200 and 300°C is exhibited in Figure 13. In accordance with the figure, the results of evaluation show that the process performed at 300°C requires more cash in payment for the equipment than the process performed at 200°C. This is because the presence of a gas compressor that must be added to the process for pressuring the gas products. The equipment costs of each unit are shown in Figure 14.



a) 200°C



b) 300°C

Figure 14. Equipment cost of unit operation

As depicted in Figure 14, it can be clearly observed that the main cost of equipment for 300°C is the compressor, which is much more expensive than other units. In the case of 200 °C, from the smallest to the largest capacities, the distillation unit used to purify and recycle chemical substances (e.g., ethanol, acetaldehyde, and ethylene glycol) is the major equipment cost of acetaldehyde production. The compressor cost of 300°C compared to the total equipment cost of 200°C is shown in Figure 15.

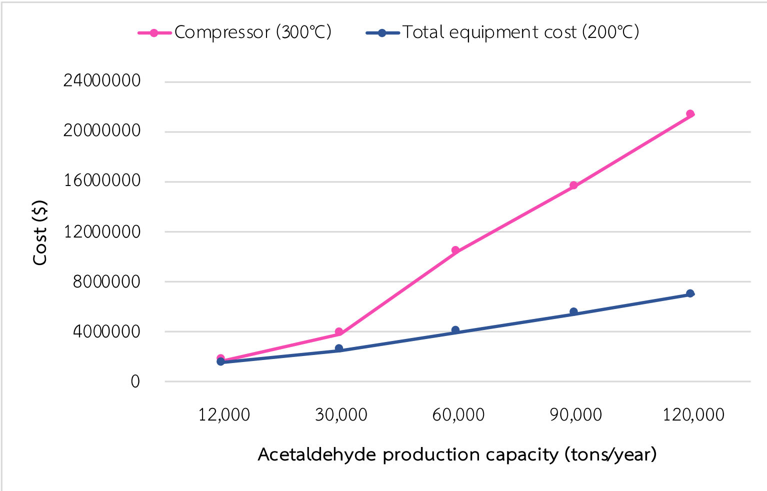


Figure 15. The comparison between the compressor cost of 300°C and total equipment cost of 200°C

According to the figure, when the process has a higher capacity, the total equipment cost for 200°C appears to be steadily rising, but is still significantly lower than the cost of a single compressor used in the acetaldehyde production process at temperature of 300°C. Thus, as mentioned above, the compressor is one of the important equipment that makes the process operating at 300°C less profitable.

In summary, a result of evaluating the relationship between economic parameters and production capacity suggests that an annual acetaldehyde production capacity of 120,000 tons is the optimum capacity since this production size has the highest percentage of IRR (The process with a higher %IRR implies that the process is more profitable and desirable).

Also, partial oxidative dehydrogenation of ethanol at 200°C is the appropriate process for acetaldehyde production when compared to another process, namely partial oxidative dehydrogenation of ethanol at 300°C. The reason is that:

1) At the same price of acetaldehyde, the process has a high %IRR and achieves a return on investment within a few years.
2) The total raw material cost and equipment cost of this process is low.
3) The process has the ability to provide a large amount of acetaldehyde.

4.4 Energy efficiency

Energy used in the process can be classified into two categories including electrical and thermal duties. The total amounts of electrical and thermal utilities for different capacities at 200 and 300°C are represented in Table 20.

Table 20. Summary of total electricity and thermal generation in both conditions

T (°C)	Energy consumption (MW)	Acetaldehyde production capacity (tons/year)				
		12,000	**30,000**	**60,000**	**90,000**	**120,000**
200	Electrical duty	1.24E-03	2.53E-03	4.45E-03	6.27E-03	8.05E-03
	Thermal duty	23.03	57.58	115.15	172.73	230.30
300	Electrical duty	1.22	3.06	6.11	9.17	12.22
	Thermal duty	7.13	17.81	35.63	53.44	71.27

Further, energy efficiency that is defined as specific energy consumption (SEC) has been calculated (See Eq. 3.2). As the term of the total electricity consumption to the total amount of acetaldehyde produced, the specific energy consumption of all cases of acetaldehyde production process is about 0.003 MJ/kg of acetaldehyde for 200°C and about 5.05 MJ/kg of acetaldehyde for 300°C. This indicates that the process occurring at temperature of 300 °C uses significantly more electricity than that of 200°C.

Figure 16 shows the estimated electricity usage of each unit at 300°C. According to the figure, it appears that the process equipment that use a lot of electricity is from a compressor which accounts for about 99% of total electricity consumption. Due to the existence of several by-products in this process, an increase in the gas pressure using a compressor prior to entering the flash drum is therefore necessary. This additional compressor can recover more than 75% of total acetaldehyde production in liquid stream coming out of the flash drum. If the compressor has not been utilized for pressuring the gases, the highest acetaldehyde yield is less than 15%.

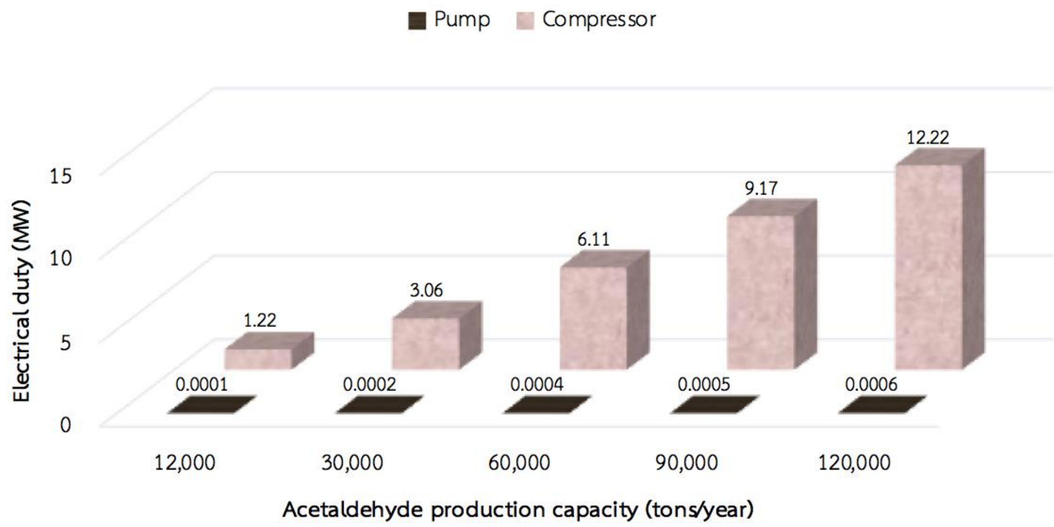
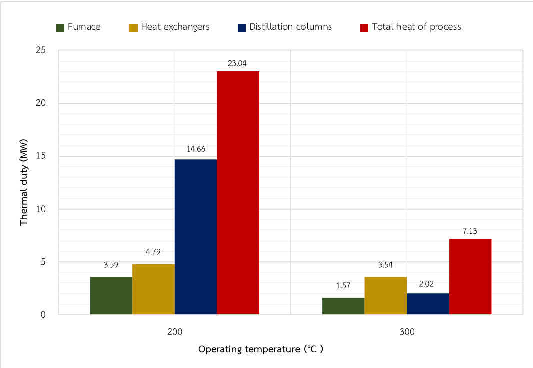


Figure 16. Electrical duties used for producing acetaldehyde at 300°C

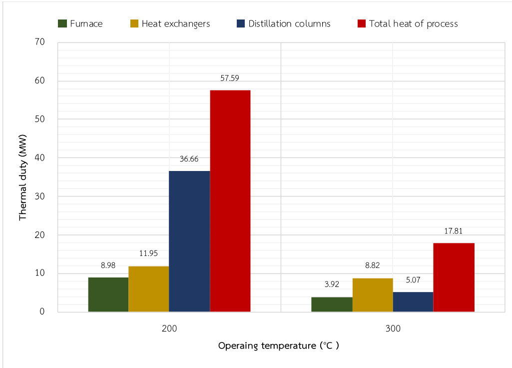
For 200°C, the total amount of electricity is only utilized by the pumps. Since the reaction yields only two different byproducts (DEE and water), over 95% of total acetaldehyde production exiting at the bottom of a phase separator can be achieved without a compressor (See Figure 11).

Regarding the thermal duty, the specific energy consumption of thermal utilities in any capacity are estimated to be about 72.32 MJ and 29.44 MJ per kilogram of acetaldehyde for operating temperature of 200 and 300°C, respectively. As mentioned above, the catalytic oxidation of ethanol at 200°C consumes enormous amounts of thermal energy compared to another condition namely 300°C.

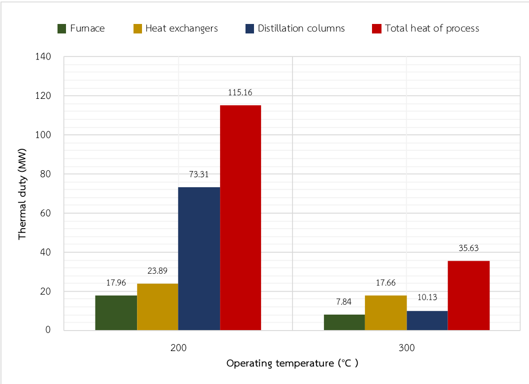
When considering the thermal duty of each unit as illustrated in Figure 17, the major use of thermal energy for 200°C is the distillation unit which accounts for 63.66% of the total thermal requirement.



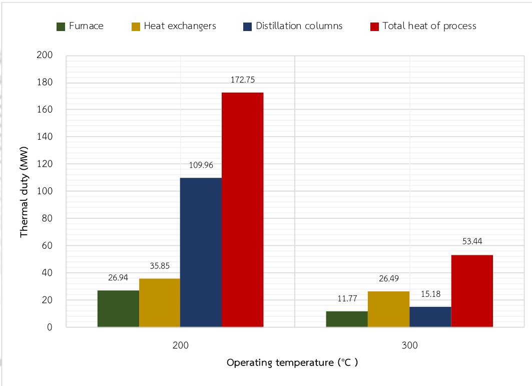
a) 12,000 tons/year



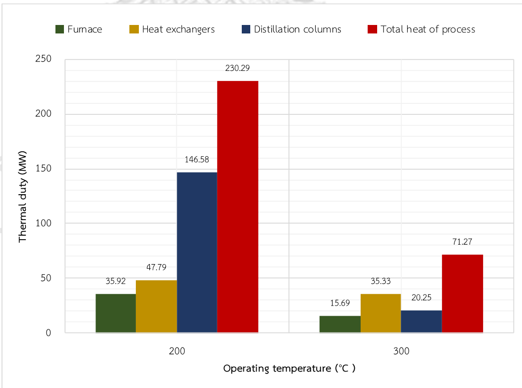
b) 30,000 tons/year



c) 60,000 tons/year



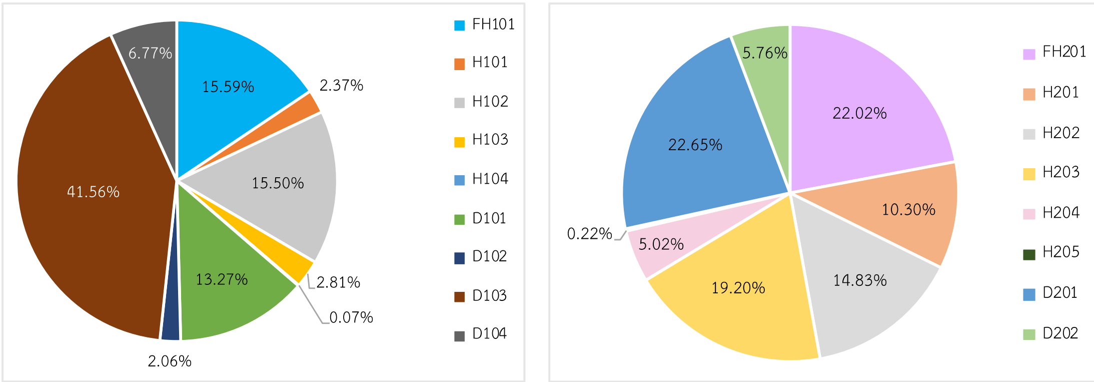
d) 90,000 tons/year



d) 120,000 tons/year

Figure 17. Thermal duties in each acetaldehyde production capacity

Since 11% conversion of ethanol is obtained at 200°C. This; therefore, leads to the large amount of thermal utilization for internal circulation of the unreacted ethanol and ethylene glycol. As depicted in Figure 18(a), nearly half of the total thermal requirement comes from the combination of thermal utilities used in ethanol (D103) and ethylene glycol recovery column (D104).



a) 200°C b) 300°C

Figure 18. The percentage of thermal duties in each unit operation

In contrast to the reaction temperature of 300°C, the partial oxidation reactor gives a high ethanol conversion (98%). This means there is no need to recycle ethanol and ethylene glycol (used in the extractive distillation). In processing ethanol to produce acetaldehyde at 300°C, the total heat used in the distillation columns is estimated to be about 28.4% as seen in Figure 18(b).

4.5 CO_2 emission assessment

According to Equation 3.3, there are two terms in the equation that are examined to calculate the net CO_2 emission of acetaldehyde production processes including CO_2 inlets and CO_2 outlets. However, the catalytic oxidation reactions take place without the utilization of CO_2. Thus, the net CO_2 emission of this study is only computed in term of CO_2 outlets.

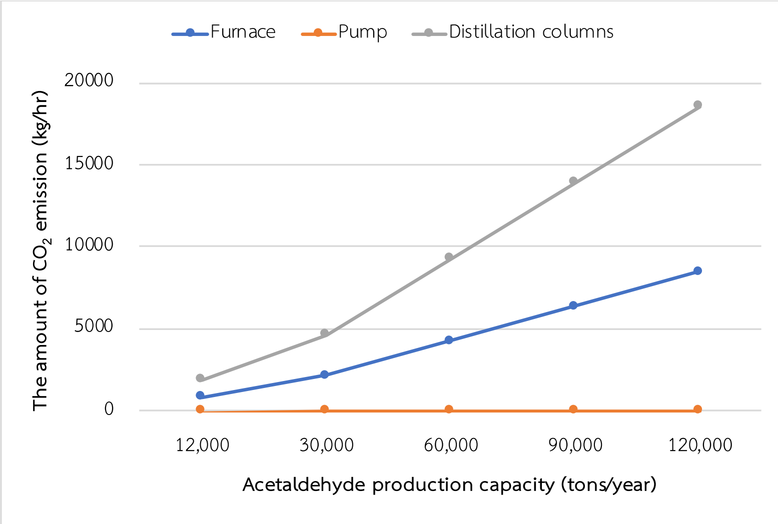
The total amounts of CO_2 released from the process are mainly obtained by 1) the chemical reaction and 2) by the usage of process utilities that is considered as direct and indirect emissions, respectively. Table 21 shows the amount of CO_2 generated in each production capacity of acetaldehyde.

Table 21. Summary of all direct and indirect CO_2 emitted into the atmosphere of both processes

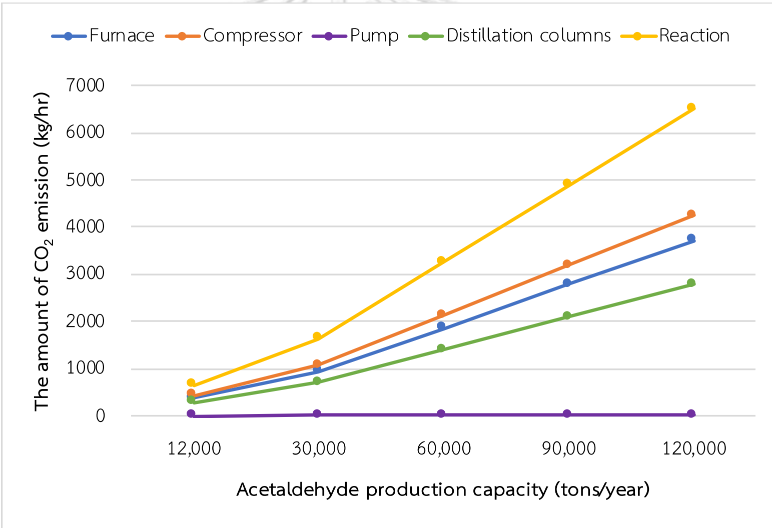
T (°C)	ACT production capacity (tons/year)	Outlet CO_2		Net CO_2 emissions (kg_{CO_2}/hr)
		Direct outlet (kg_{CO_2}/hr)	Indirect outlet (kg_{CO_2}/hr)	
200	12,000	-	2,709.81	2,709.81
	30,000	-	6,774.40	6,774.40
	60,000	-	13,548.57	13,548.57
	90,000	-	20,322.92	20,322.92
	120,000	-	27,096.89	27,096.89
300	12,000	650.20	1,074.35	1,724.55
	30,000	1,625.50	2,685.95	4,311.45
	60,000	3,251.00	5,372.83	8,623.83
	90,000	4,876.51	8,056.87	12,933.38
	120,000	6,502.01	10,743.27	17,245.28

After that, the released CO_2 per 1 kilogram of producing acetaldehyde is determined for comparative purpose. According to the table above, the amounts of CO_2 exiting the process are estimated to be about 2.36 kg_{CO_2}/kg_{ACT} for 200°C and 1.98 kg_{CO_2}/kg_{ACT} for 300°C. Referring to the previously mentioned, it has been found that the total CO_2 emissions at operating temperature of 200°C are higher than that of 300°C.

Figure 19 shows the amount of CO_2 in each CO_2 emission source. For partial oxidation of ethanol at temperature of 200°C, the amounts of CO_2 obtained from the distillation units accounts for about 68.60% of the total CO_2 emission. This is because the low ethanol conversion in the case of 200°C that contributes to the increased number of distillation columns for ethanol and ethylene glycol recovery. As a result, the large amount of process utility is required. In other words, the larger the utility usage, the larger the amount of CO_2 emissions.



a) 200°C



b) 300°C

Figure 19. The amounts of CO_2 generated from each unit

For another process (300°C), just 16.20% of the total CO_2 emission is obtained from the distillation columns since the reaction provides 98% ethanol conversion. Therefore, the process utilities of distillation unit are used in smaller quantities. However, the compressor has higher CO_2 emissions. Because of the formation of various types of by-products, the gas compressor must be added to the process. The percentage of indirect CO_2 emission caused by the compressor is approximately 24.60%.

In addition, the large amount of CO_2 produced in this process also comes directly from the chemical reaction. Since 21.5% selectivity of CO_2 is achieved in vapor-phase oxidation of ethanol at 300°C, about 37.70% of the total CO_2 emissions are generated by their reaction.

4.6 Heat recovery

Heat recover has been conducted in this work also. The units involved in the heat recovery are the heat exchanger H101 and H202 in the acetaldehyde production process at 200 and 300°C, respectively.

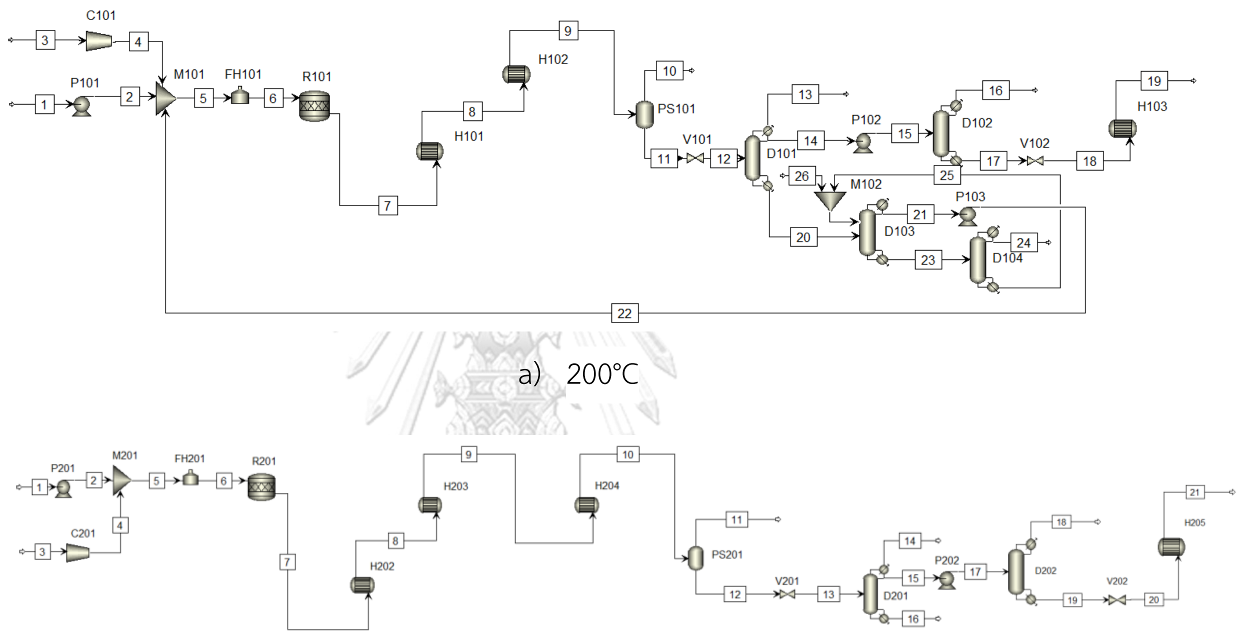
The heat exchanger H101 in the process operating at 200°C is used to reduce the temperature of stream 5^{th} from 200 to 120.89°C. The heat released by this process stream is absorbed by boiler feed water (BFW) available at 110.89°C. The water is vaporized to a saturated steam which can be further used as the source of reboiler heat in the distillation column D101.

As the same as the heat exchanger H202 in the process operating at 300°C, this equipment is served to cool down the stream temperature (stream 7^{th}) and exited H202 at about 139°C. Regarding the process utility provided for H202, the type of utility is BFW. The heat obtained from stream 7^{th} is utilized to generate the hot steam needed for reboiler in the distillation column D201. The usage of the heating utility generated from the heat exchanger to the distillation unit can decrease the utility costs of the manufacturing process.

4.7 Recommendation for future work

As appeared in Figure 16, the compressor cost dramatically impacts the budget. Therefore, the simulation of acetaldehyde production processes that have an operating pressure of 10 bar is presented since it is expected that the catalytic oxidation reaction performed at high pressure may enhance the profitability of processes. Please note that the ethanol oxidation reactor only changes the operating pressure. For the reaction temperature, the values of process parameters (i.e., conversion and selectivity), and the operating pressure and structure of distillation units in both acetaldehyde production processes (at 200 and 300°C), all of these are assumed to be unchanged.

In this work, partial oxidative dehydrogenation of ethanol having two different operating temperatures with an acetaldehyde production capacity of 120,000 tons/year (at the reactor outlet stream) is the representative of simulating at pressure of 10 bar. The process flow diagrams of manufacturing acetaldehyde at 10 bar pressure are shown in Figure 20.



a) 200°C

b) 300°C

Figure 20. Process flow diagrams of acetaldehyde production at 10 bar

Under the reaction pressure of 10 bar, the profitability of acetaldehyde production process at 300°C is improved, which can be seen from Table 22. According to the table, the results show that the percentage of IRR in the case of operating at 10 bar is higher than that of operating at 1 atm for 300°C. This is because the compressor that has lower equipment cost. The cost of a gas compressor will depend on the inlet feed flow rate of substances – that is the higher the inlet gas flow rate, the higher the compressor cost. For the production rate of acetaldehyde, both conditions have the same rate.

Table 22. Economic analysis results of vapor-phase ethanol oxidation reactions at pressure of 1.01325 and 10 bar

T (°C)	P (bar)	PI	POP	%IRR	Inlet capacity (m^3/hr)	Compressor cost ($)	Production rate (tons/year)
200	1.01325	1.47	1.77	166.26	-	-	111,894.13
	10	1.44	1.88	147.01	16,755.62	2,454,200	104,313.95
300	1.01325	1.08	4.95	40.29	103,405.01	21,345,000	85,031.19
	10	1.12	3.86	52.50	60,688.06	10,562,000	85,031.19

In the case of operating at 200°C, the process is less profitable when the reaction pressure is 10 bar. The reasons are as follows:

1) The addition of a compressor to the process that results in higher equipment cost.

   The air in Earth's atmosphere that contains 20.95% oxygen is utilized to conduct the partial oxidative dehydrogenation reaction in this work. Thus, a compressor is employed to increase the pressure of gases.

2) The lower production rate of acetaldehyde that leads to a decrease in total product sales.

   In the distillation column D101, the partial condenser is processed to condense the overhead product as well as released any remaining gas. The distillate vapor fraction for the reaction operating at atmospheric pressure is only 0.01 because of a small quantity of light components (e.g., O_2, N_2, Ar, and CO_2) in stream 11th (Figure 5).

   However, when the catalytic reactor performs at pressure of 10 bar, the stream 12th appeared in Figure 20(a) has more light components. As such, the fraction of the vapor phase for D101 in this process increases to 0.1 which causes a certain amount of acetaldehyde to be lost to the gas stream 13th. If the distillate vapor fraction of 0.01 is set, the condenser temperature goes below 0°C.

In summary, at the reaction pressure of 10 bar, the process that can be increased profitability is partial oxidative dehydrogenation of ethanol with operating temperature of 300°C.

CHAPTER V
CONCLUSION

In engine applications, an attractive alternative fuel is gasohol, the fuel mixture of bioethanol and gasoline. Bioethanol can be produced by the fermentation of plant materials which is one of renewable energy sources that can reduce CO_2 emitted from fossil fuel combustion. However, the involvement of battery electric vehicles (BEV) may decrease ethanol demand for gasohol in the future. Therefore, in this work, the utilization of ethanol to produce acetaldehyde via oxidative dehydrogenation reaction is processed due to the many benefits of acetaldehyde and its higher price.

In this work, the process simulation and economic analysis of acetaldehyde production is conducted by Aspen Plus. The experiment results obtained from published literatures regarding partial oxidative dehydrogenation of ethanol using V-Zr-La/SBA-15 as the catalyst under two different operating temperature (i.e., 200 and 300 °C) with constant pressure of 1 atm are used as input data to simulate the acetaldehyde production process. For the production sizes of simulating the manufacturing process, it is divided into five capacities including 12,000, 30,000, 60,000, 90,000, and 120,000 tons of acetaldehyde per year.

At the same price of acetaldehyde, the optimum capacity is an acetaldehyde production capacity of 120,000 tons/year since this proposed capacity provides the highest %IRR.

Further, regarding the determination of which process is most suitable for acetaldehyde synthesis from ethanol, the appropriate process for producing acetaldehyde is partial oxidative dehydrogenation of ethanol at 200°C, primarily because of its higher %IRR and shorter POP when compared to another process, namely partial oxidative dehydrogenation of ethanol at 300°C. The reasons that the process operating at temperature of 200°C earns higher profits than that of 300°C are as follows: 1) the process consumes less amount of ethanol, 2) the process has the potential to produce the larger amount of acetaldehyde, and 3) the total costs of equipment for this process is lower.

In terms of energy requirement, the large amounts of electric utilities are used by the process performed at 300°C due to the addition of a gas compressor to the process. For the thermal duty, the process performed at 200°C consumes the large amounts of thermal utilities. Since a low ethanol conversion is achieved in this process, the increased number of distillation column for the recycling of unreacted ethanol is necessary. As a result, thermal utilities are loaded into the process in large quantities.

Furthermore, because of its low conversion of ethanol in the case of operating at 200°C, this process also has high CO_2 emissions. Please note that if the large utilities are utilized, the high level of CO_2 emissions is received.

Regarding the heat recovery, the heat released from the reduction of temperature in stream 5^{th} for the process operating at 200°C and in stream 7^{th} for the process operating at 300°C is used to generate a saturated steam, the heat source required for reboiler in the distillation column D101 and D201, respectively. This leads to decrease in demand for the external utility.

For the future work, it has been found that the existence of a compressor (at the back of a reactor) significantly reduces the process profitability. Thus, high-pressure experiments may be used to enhance the profits.

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APPENDIX

APPENDIX A FEEDSTOCK ESTIMATION

For the simulation of acetaldehyde production process, acetaldehyde produced by partial oxidative dehydrogenation of ethanol over V-Zr-La/SBA-15 catalyst at different conditions (i.e., 200 and 300°C) is used in this work. The experimental results obtained from this reaction are represented in accordance with Table A1.

Table A1. Conversion and selectivity in partial oxidative dehydrogenation of ethanol using V-Zr-La/SBA-15 catalyst at 200 and 300°C

T (°C)	P (atm)	Ethanol conversion (%)	Selectivity (%)				
			ACT*	DEE	CO_2	CO	C_2H_4
200	1	11	99	1	-	-	-
300	1	98	41	1	21.5	21.5	15

* ACT: Acetaldehyde

Further, according to the given information above, the process parameters such as conversion and selectivity are used to estimate the values of the mass flow rates of 99.5 wt% ethanol and air required for acetaldehyde preparation. Summary of the quantities of both reactants that need to be brought into the acetaldehyde production processes is shown in Table 10 (See Chapter 3, Section 3.2)

Regarding the calculated results as provided in Table 10, the next section will represent the calculation examples of each process based on the fixed acetaldehyde production capacity of 120,000 tons/year (or 2727.27 x 10^6 mol/year) at reactor outlet stream.

$$\frac{120{,}000\ \frac{\text{tons}}{\text{year}} \times \frac{10^6}{1}\ \frac{\text{g}}{\text{tons}}}{44\ \frac{\text{g}}{\text{mol}}} = 2727.27 \times 10^6\ \frac{\text{mol}}{\text{year}}$$

Please note that molar basis of overall product is 100 mol/year.

A.1 Acetaldehyde production over V-Zr-La/SBA-15 catalyst at reaction temperature of 200°C and atmospheric pressure

Finding the amount of ethanol and air used for producing acetaldehyde and diethyl ether (DEE).

From stoichiometric coefficients in partial oxidative dehydrogenation of ethanol, we get:

- Oxidative dehydrogenation of ethanol towards acetaldehyde (99% selectivity of ACT)

$$C_2H_5OH + 0.5O_2 \longrightarrow CH_3CHO + H_2O$$

	C_2H_5OH	$0.5O_2$	CH_3CHO	H_2O	
Molecular weight	46	32	44	18	$\frac{g}{mol}$
Mole	99	49.50	99	99	$\frac{mol}{year}$
Mass	4,554	1,584	4,356	1,782	$\times 10^{-6}\ \frac{tons}{year}$

- Dehydrogenation of ethanol towards diethyl ether (1% selectivity of DEE)

$$2C_2H_5OH \longrightarrow C_2H_5OC_2H_5 + H_2O$$

	$2C_2H_5OH$	$C_2H_5OC_2H_5$	H_2O	
Molecular weight	46	74	18	$\frac{g}{mol}$
Mole	2	1	1	$\frac{mol}{year}$
Mass	92	74	18	$\times 10^{-6}\ \frac{tons}{year}$

On a mass basis, about $4,356 \times 10^{-6}$ tons per year of acetaldehyde is produced. Thus, if acetaldehyde has increased production to 120,000 tons per year, the total mass and molar flow rates of each substance such as ethanol, oxygen, DEE and water that utilize can be computed as follow:

$$\text{Ethanol} = (\text{Ethanol})_{ACT} + (\text{Ethanol})_{DEE}$$

$$= \frac{((4,554 + 92) \times 10^{-6}) \times 120,000}{(4,356 \times 10^{-6})} \frac{tons}{year}$$

$$= 127,988.98 \frac{tons}{year}$$

$$\text{Oxygen} = \frac{(1{,}584 \times 10^{-6}) \times 120{,}000}{(4{,}356 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 43{,}636.36 \frac{\text{tons}}{\text{year}}$$

$$\text{DEE} = \frac{(74 \times 10^{-6}) \times 120{,}000}{(4{,}356 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 2{,}038.57 \frac{\text{tons}}{\text{year}}$$

$$\text{Water} = (\text{Water})_{ACT} + (\text{Water})_{DEE}$$

$$= \frac{((1{,}782 + 18) \times 10^{-6}) \times 120{,}000}{(4{,}356 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 49{,}586.78 \frac{\text{tons}}{\text{year}}$$

In catalytic oxidation of ethanol towards acetaldehyde at operating temperature of 200°C, the amount of oxygen used in this reaction = 1,363.64 x 10^6 mol/year.

However, the air in Earth's atmospheric consisting of approximately 20.95 mol% oxygen, 78.08 mol% nitrogen, 0.93 mol% argon, and 0.04 mol% carbon dioxide is used an unlimited oxygen supply in this work. Thus, total air requirement = $\frac{(1{,}363.64 \times 10^6) \times 100}{20.95}$ = 6,509.00 x 10^6 mol/year = 188,531.35 tons/year. Please note that molecular weight of air is 28.9647 g/mol.

For ethanol, the amount of ethanol consumed in both reactions is about 127,988.98 tons/year at 11% conversion of ethanol. Therefore, the total feed rate of pure ethanol = $\frac{100 \times 127{,}988.98}{11}$ = 1,163,536.19 tons/year. However, this work uses a 99.5 wt% grade ethanol. As such, the actual feed of ethanol = $\frac{1{,}163{,}536.19}{0.995}$ = 1,169,383.10 tons/year.

A.2 Acetaldehyde production over V-Zr-La/SBA-15 catalyst at reaction temperature of 300°C and atmospheric pressure

Finding the amount of ethanol and air used for producing acetaldehyde, diethyl ether (DEE), carbon dioxide, carbon monoxide, and ethylene.

From stoichiometric coefficients in partial oxidative dehydrogenation of ethanol, we get:

- Oxidative dehydrogenation of ethanol towards acetaldehyde (41% selectivity of ACT)

	C_2H_5OH	+ $0.5O_2$ →	CH_3CHO	+ H_2O	
Molecular weight	46	32	44	18	$\frac{g}{mol}$
Mole	41	20.5	41	41	$\frac{mol}{year}$
Mass	1,886	656	1,804	738	$\times 10^{-6}\ \frac{tons}{year}$

- Dehydrogenation of ethanol towards diethyl ether (1% selectivity of DEE)

	$2C_2H_5OH$ →	$C_2H_5OC_2H_5$	+ H_2O	
Molecular weight	46	74	18	$\frac{g}{mol}$
Mole	2	1	1	$\frac{mol}{year}$
Mass	92	74	18	$\times 10^{-6}\ \frac{tons}{year}$

- Oxidative dehydrogenation of ethanol towards carbon dioxide (21.5% selectivity of CO_2)

	C_2H_5OH	+ $3O_2$ →	$2CO_2$	+ $3H_2O$	
Molecular weight	46	32	44	18	$\frac{g}{mol}$
Mole	10.75	32.25	21.50	32.25	$\frac{mol}{year}$
Mass	494.50	1,032	946	580.50	$\times 10^{-6}\ \frac{tons}{year}$

- Oxidative dehydrogenation of ethanol towards carbon monoxide (21.5% selectivity of CO)

	C_2H_5OH	+ $2O_2$ →	$2CO$	+ $3H_2O$	
Molecular weight	46	32	28	18	$\frac{g}{mol}$
Mole	10.75	21.50	21.50	32.25	$\frac{mol}{year}$
Mass	494.50	688	602	580.50	$\times 10^{-6}\ \frac{tons}{year}$

- Dehydrogenation of ethanol towards ethylene (15% selectivity of C_2H_4)

	C_2H_5OH →	C_2H_4	+ H_2O	
Molecular weight	46	28	18	$\frac{g}{mol}$
Mole	15	15	15	$\frac{mol}{year}$
Mass	690	420	270	$\times 10^{-6}\ \frac{tons}{year}$

On a mass basis, about 1,804 x 10^{-6} tons per year of acetaldehyde is produced. Thus, if acetaldehyde has increased production to 120,000 tons per year, the total mass and molar flow rates of each substance such as ethanol, oxygen, DEE and water that utilize can be computed as follow:

$$\text{Ethanol} = (\text{Ethanol})_{ACT} + (\text{Ethanol})_{DEE} + (\text{Ethanol})_{CO_2} + (\text{Ethanol})_{CO} + (\text{Ethanol})_{C_2H_4}$$

$$= \frac{((1{,}886 + 92 + 494.50 + 494.50 + 690) \times 10^{-6}) \times 120{,}000}{(1{,}804 \times 10^{-6})} \frac{tons}{year}$$

$$= 243{,}259.42\ \frac{tons}{year}$$

$$\text{Oxygen} = (\text{Oxygen})_{ACT} + (\text{Oxygen})_{CO_2} + (\text{Oxygen})_{CO}$$

$$= \frac{((656 + 1{,}032 + 688) \times 10^{-6}) \times 120{,}000}{(1{,}804 \times 10^{-6})} \frac{tons}{year}$$

$$= 158{,}048.78\ \frac{tons}{year}$$

$$\text{DEE} = \frac{(74 \times 10^{-6}) \times 120{,}000}{(1{,}804 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 4{,}922.39 \frac{\text{tons}}{\text{year}}$$

$$CO_2 = \frac{(946 \times 10^{-6}) \times 120{,}000}{(1{,}804 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 62{,}926.83 \frac{\text{tons}}{\text{year}}$$

$$\text{CO} = \frac{(602 \times 10^{-6}) \times 120{,}000}{(1{,}804 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 40{,}044.35 \frac{\text{tons}}{\text{year}}$$

$$\text{Ethylene} = \frac{(420 \times 10^{-6}) \times 120{,}000}{(1{,}804 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 27{,}937.92 \frac{\text{tons}}{\text{year}}$$

$$\text{Water} = (\text{Water})_{ACT} + (\text{Water})_{DEE} + (\text{Water})_{CO_2} + (\text{Water})_{CO} + (\text{Water})_{C_2H_4}$$

$$= \frac{((738 + 18 + 580.50 + 580.50 + 270) \times 10^{-6}) \times 120{,}000}{(1{,}804 \times 10^{-6})} \frac{\text{tons}}{\text{year}}$$

$$= 145{,}476.72 \frac{\text{tons}}{\text{year}}$$

In catalytic oxidation of ethanol towards acetaldehyde at operating temperature of 300°C, the amount of oxygen used in this reaction = 4,939.02 x 10^6 mol/year.

However, the air in Earth's atmospheric consisting of approximately 20.95 mol% oxygen, 78.08 mol% nitrogen, 0.93 mol% argon, and 0.04 mol% carbon dioxide is used an unlimited oxygen supply in this work. Thus, total air requirement = $\frac{(4{,}939.02 \times 10^{6}) \times 100}{20.95}$ = 23,575.30 x 10^6 mol/year = 682,851.36 tons/year. Please note that molecular weight of air is 28.9647 g/mol.

For ethanol, the amount of ethanol consumed in five reactions is about 243,259.42 tons/year at 98% conversion of ethanol. Therefore, the total feed rate of pure ethanol = $\frac{100 \times 243,259.42}{98}$ = 248,223.90 tons/year. However, this work uses a 99.5 wt% grade ethanol. As such, the actual feed of ethanol = $\frac{248,223.90}{0.995}$ = 249,471.26 tons/year.

APPENDIX B REACTOR SIZING

In this work, packed bed reactor is selected for achieving the vapor phase oxidative dehydrogenation of ethanol to acetaldehyde over V-Zr-La/SBA-15 catalyst. Accordingly, the geometric parameters, such as the diameter and length of the reactor as well as the length of catalyst bed, have been calculated to evaluate the economic values of processes. Table B1 represents all calculated values of such parameters under five different production capacities of acetaldehyde.

Table B1. Summary of each geometric parameter values for techno-economic analysis

T (°C)	Capacity (tons/year)	D (m)	W_{cat} (kg)	V_{bed} (m^3)	L_{bed} (m)	L_{react} (m)
200	12,000	1.7761	525.83	7.85	3.1676	4.1096
	30,000	2.8083	1,314.56	19.62		
	60,000	3.9715	2,629.11	39.24		
	90,000	4.8641	3,943.66	58.86		
	120,000	5.6166	5,258.22	78.48		
300	12,000	0.8204	112.18	1.67	3.1676	4.1096
	30,000	1.2971	280.44	4.19		
	60,000	1.8344	560.88	8.37		
	90,000	2.2467	841.32	12.56		
	120,000	2.5942	1,121.77	16.74		

Example of calculation: Production capacity of acetaldehyde at 120,000 tons/year

The 1st step: Calculate the reactor diameter (D)

The diameter of the reactor can be computed using the formula given below:

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

Where; G = mass velocity

$\dot{m}$ = mass flow rate

D = vessel diameter

For partial oxidation of ethanol at 200°C with an annual acetaldehyde production capacity of 120,000 tons, ethanol flow rate is about 33.4481 kg/s. In addition, mass velocity of 1.35 $\frac{kg}{m^2 \cdot s}$ is preferable since the reactions are carried out in a vapor-phase packed bed reactor. Thus, we get;

$$\text{Diameter calculated (D)} = \left(\frac{4 \times 33.4481 \frac{kg}{s}}{1.35 \frac{kg}{m^2 \cdot s} \times \pi} \right)^{\frac{1}{2}}$$

$$= 5.6166 \text{ m}$$

The 2nd step: Find the catalyst weight (W_{cat})

As referred in the literature, weight hourly space velocity (WHSV) of this process is 22.9 ($g_{ethanol}g_{cat}^{-1}$) h^{-1}.

$$\text{WHSV} = \frac{\dot{m}}{W_{cat}}$$

From the above equation, the mass of catalyst is as follows;

$$\text{Catalyst weight } (W_{cat}) = \frac{33.4481 \frac{kg_{ethanol}}{s} \times \frac{3{,}600 \text{ s}}{1 \text{ h}}}{22.9 \frac{kg_{ethanol}}{kg_{cat} \cdot h}}$$

$$= 5{,}258.22 \text{ } kg_{cat}$$

The 3rd step: Calculate the volume of catalyst bed (V_{bed})

In this work, V-Zr-La/SBA-15 catalyst prepared by hydrothermal method is used to catalyze ethanol into acetaldehyde with a bulk density of 0.067 g/cm^3.

$$\text{Catalyst bed volume } (V_{bed}) = \frac{W_{cat}}{\rho_b}$$

$$= \frac{5{,}258.22 \text{ } kg_{cat}}{0.067 \frac{g_{cat}}{cm^3} \times \frac{1 \text{ } kg_{cat}}{1{,}000 \text{ } g_{cat}} \times \frac{10^6 \text{ } cm^3}{1 \text{ } m^3}}$$

$$= 78.48 \text{ } m^3$$

The 4th step: Calculate the length of the reactor (L_{react}) and catalyst bed (L_{bed})

For the catalyst bed length

$$V_{bed} = \frac{\pi D^2 L_{bed}}{4}$$

$$L_{bed} = \frac{4 \times 78.48\ m^3}{\pi \times (5.6166\ m)^2}$$

$$= 3.1676\ m$$

For the reactor length

$$L_{react} = L_{bed} + 0.942$$

$$= 3.1676 + 0.942$$

$$= 4.1096\ m$$

APPENDIX C STREAM RESULTS

Table C1. Stream results of acetaldehyde production capacity of 12,000 tons/year at 200℃

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	°C	30	30	52.49	200	200	120.89	45
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Molar Vapor Fraction		0	1	0.3023	1	1	1	0.2262
Mole Flows	kmol/hr	31.669	67.3585	331.958	331.958	346.047	346.047	346.047
Mass Flows	tons/year	13988.8	18853.1	135792	135792	135792	135792	135792
Ethanol	tons/year	13918.9	0	116354	116354	103555	103555	103555
Oxygen	tons/year	0	4363.31	4363.31	4363.31	7.2248	7.2248	7.2248
Nitrogen	tons/year	0	14236.6	14236.6	14236.6	14236.6	14236.6	14236.6
Argon	tons/year	0	241.811	241.811	241.811	241.811	241.811	241.811
Carbon dioxide	tons/year	0	11.458	11.458	11.458	11.458	11.458	11.458
Acetaldehyde	tons/year	0	0	30.6433	30.6433	12024.8	12024.8	12024.8
Diethyl ether	tons/year	0	0	0.5865	0.5865	206.516	206.516	206.516
Water	tons/year	69.9441	0	546.192	546.192	5501.18	5501.18	5501.18
Ethylene glycol	tons/year	0	0	7.2785	7.2785	7.2785	7.2785	7.2785

Table C1. Stream results of acetaldehyde production capacity of 12,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	10	10	10	10.12	31.06	31.06	31.14
Pressure	bar	1.01325	1.01325	1.01325	2.34	2	2	2.54
Molar Vapor Fraction		0.1607	1	0	0	1	0	0
Mole Flows	kmol/hr	346.047	55.6219	290.425	290.425	0.2784	27.5658	27.5658
Mass Flows	tons/year	135792	15503.1	120289	120289	108.228	11755.7	11755.6747
Ethanol	tons/year	103555	594.667	102961	102961	2.8604E-03	10.2923	10.29225
Oxygen	tons/year	7.2248	7.2066	0.0181	0.0181	0.0158	2.3555E-03	0.00236
Nitrogen	tons/year	14236.6	14215.7	20.8852	20.8852	19.118	1.7672	1.7672
Argon	tons/year	241.811	241.168	0.6431	0.6431	0.6373	0.0058	0.0058
Carbon dioxide	tons/year	11.458	11.0275	0.4305	0.4305	0.3661	0.0643	0.0643
Acetaldehyde	tons/year	12024.8	369.062	11655.7	11655.7	85.9281	11539.2	11539.1645
Diethyl ether	tons/year	206.516	32.3658	174.15	174.15	2.0745	171.489	171.4891
Water	tons/year	5501.18	31.9421	5469.24	5469.24	0.08515	32.8892	32.8892
Ethylene glycol	tons/year	7.2785	1.1648E-05	7.2785	7.2785	1.1507E-20	1.198E-14	1.1980E-14

Table C1. Stream results of acetaldehyde production capacity of 12,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	41.52	47.20	40.66	30	100.89	96.52	78.24
Pressure	bar	2.2	2.54	2.05	2.05	2.34	2	1.01325
Molar Vapor Fraction		1	0	0.0365	0	0	0	0.0716
Mole Flows	kmol/hr	1.2347	26.3311	26.3311	26.3311	262.5806	232.9313	232.9310
Mass Flows	tons/year	566.1819	11189.493	11189.493	11189.493	108425.27	102950.49	102950.331
Ethanol	tons/year	1.7984E-12	10.2923	10.2923	10.2923	102950.49	102435.73	102435.575
Oxygen	tons/year	0.00236	3.36E-31	3.36E-31	3.36E-31	1.13E-17	0	0
Nitrogen	tons/year	1.7672	1.75E-30	1.75E-30	1.75E-30	1.76E-15	0	0
Argon	tons/year	0.0058	4.83E-46	4.83E-46	4.83E-46	5.77E-16	0	0
Carbon dioxide	tons/year	0.0643	2.83E-31	2.83E-31	2.83E-31	3.85E-12	0	0
Acetaldehyde	tons/year	461.5666	11077.5979	11077.5979	11077.5979	30.6433	30.6433	30.6433
Diethyl ether	tons/year	102.7290	68.7601	68.7601	68.7601	0.5865	0.5865	0.5865
Water	tons/year	0.0466	32.8426	32.8426	32.8426	5436.2643	476.2462	476.2474
Ethylene glycol	tons/year	0	0	0	0	7.2785	7.2794	7.2785

Table C1. Stream results of acetaldehyde production capacity of 12,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	22	23	24	25	26
Temperature	°C	159.74	110.92	227.33	227.40	227.33
Pressure	bar	2.34	2	2.34	2.34	2.34
Molar Vapor Fraction		0	0	0	0	2.40E-09
Mole Flows	kmol/hr	100.6629	29.6792	70.9837	0.03	71.0137
Mass Flows	tons/year	48060.638	5492.7701	42567.868	17.9928	42585.861
Ethanol	tons/year	514.7602	514.7599	3.1171E-04	0	3.1171E-04
Oxygen	tons/year	0	0	0	0	0
Nitrogen	tons/year	0	0	0	0	0
Argon	tons/year	0	0	0	0	0
Carbon dioxide	tons/year	0	0	0	0	0
Acetaldehyde	tons/year	7.7251E-06	7.7251E-06	3.4472E-12	0	3.4481E-12
Diethyl ether	tons/year	2.4693E-07	2.4693E-07	9.4448E-13	0	9.4709E-13
Water	tons/year	4962.1544	4960.018	2.1363	0	2.1363
Ethylene glycol	tons/year	42583.723	17.9922	42565.731	17.9928	42583.724

Table C2. Stream results of acetaldehyde production capacity of 30,000 tons/year at 200℃

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	℃	30	30	52.49	200	200	120.89	45
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Molar Vapor Fraction		0	1	0.3023	1	1	1	0.2262
Mole Flows	kmol/hr	79.171	168.3963	829.8918	829.8918	865.1122	865.1122	865.1122
Mass Flows	tons/year	34971.371	47132.84	339478.76	339478.76	339478.76	339478.76	339478.757
Ethanol	tons/year	34796.514	0	290884.18	290884.18	258886.92	258886.92	258886.922
Oxygen	tons/year	0	10908.27	10908.27	10908.27	18.131833	18.131833	18.1318
Nitrogen	tons/year	0	35591.397	35591.397	35591.397	35591.397	35591.397	35591.3972
Argon	tons/year	0	604.5276	604.5276	604.5276	604.5276	604.5276	604.5276
Carbon dioxide	tons/year	0	28.6449	28.6449	28.6449	28.6449	28.6449	28.6449
Acetaldehyde	tons/year	0	0	76.6084	76.6084	30061.7960	30061.7960	30061.7960
Diethyl ether	tons/year	0	0	1.4661	1.4661	516.2861	516.2861	516.2861
Water	tons/year	174.8569	0	1365.4654	1365.4654	13752.8562	13752.8562	13752.8562
Ethylene glycol	tons/year	0	0	18.1958	18.1958	18.1958	18.1958	18.1958

Table C2. Stream results of acetaldehyde production capacity of 30,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	10	10	10	10.09	31.06	31.06	31.14
Pressure	bar	1.01325	1.01325	1.01325	2.34	2	2	2.54
Molar Vapor Fraction		0.1607	1	0	0	1	0	0
Mole Flows	kmol/hr	865.1122	139.0550	726.0572	726.0572	0.6961	68.9141	68.9141
Mass Flows	tons/year	339478.757	38757.855	300720.902	300720.902	270.5674	29388.983	29388.983
Ethanol	tons/year	258886.922	1486.6692	257400.253	257400.253	0.0072	25.7302	25.7302
Oxygen	tons/year	18.1318	18.0863	0.0455	0.0455	0.0396	0.0059	0.0059
Nitrogen	tons/year	35591.3972	35539.185	52.2126	52.2126	47.7948	4.4178	4.4178
Argon	tons/year	604.5276	602.91997	1.6077	1.6077	1.5932	0.0145	0.0145104
Carbon dioxide	tons/year	28.6449	27.568768	1.0761	1.0761	0.9153	0.16085	0.16085
Acetaldehyde	tons/year	30061.7960	922.6564	29139.1396	29139.1396	214.81835	28847.713	28847.713
Diethyl ether	tons/year	516.2861	80.9145	435.3716	435.3716	5.1862	428.7193	428.7193
Water	tons/year	13752.8562	79.8553	13673.001	13673.001	0.2129	82.2214	82.2214
Ethylene glycol	tons/year	18.1958	2.9120E-05	1.8196E+01	1.8196E+01	2.8762E-20	2.9943E-14	2.9943E-14

Table C2. Stream results of acetaldehyde production capacity of 30,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	41.52	47.20	40.66	30	100.89	96.52	78.24
Pressure	bar	2.2	2.54	2.05	2.05	2.34	2	1.01325
Molar Vapor Fraction		1	0	0.0365	0	0	0	0.0716
Mole Flows	kmol/hr	3.0867	65.8273	65.8273	65.8273	656.4470	582.3244	582.3245
Mass Flows	tons/year	1415.4432	27973.54	27973.54	27973.54	271061.35	257374.51	257374.5465
Ethanol	tons/year	4.50E-12	25.7302	25.7302	25.7302	257374.52	256087.63	256087.668
Oxygen	tons/year	0.0059	8.435E-31	8.435E-31	8.435E-31	2.825E-17	0	0
Nitrogen	tons/year	4.4178	4.374E-30	4.374E-30	4.374E-30	4.402E-15	0	0
Argon	tons/year	0.0145	1.207E-45	1.207E-45	1.207E-45	1.4414E-15	0	0
Carbon dioxide	tons/year	0.16085	7.0774E-31	7.0774E-31	7.0774E-31	9.6242E-12	0	0
Acetaldehyde	tons/year	1153.9085	27693.804	27693.804	27693.804	76.6084	76.6084	76.6084
Diethyl ether	tons/year	256.8191	171.9002	171.9002	171.9002	1.4660705	1.4661	1.4661
Water	tons/year	0.1165	82.1049	82.1049	82.1049	13590.567	1190.6084	1190.6086
Ethylene glycol	tons/year	0	0	0	0	18.1957	18.195601	18.1958

Table C2. Stream results of acetaldehyde production capacity of 30,000 tons/year at 200℃ (Cont'd)

Stream No.	Unit	22	23	24	25	26
Temperature	℃	159.74	110.92	227.33	227.40	227.33
Pressure	bar	2.34	2	2.34	2.34	2.34
Molar Vapor Fraction		0	0	0	0	3.30E-09
Mole Flows	kmol/hr	251.6536	74.1946	177.4590	0.0720	177.5310
Mass Flows	tons/year	120149.4584	13730.0281	106419.4303	43.1826	106462.6125
Ethanol	tons/year	1286.8883	1286.8875	7.8185E-04	0	7.8186E-04
Oxygen	tons/year	0	0	0	0	0
Nitrogen	tons/year	0	0	0	0	0
Argon	tons/year	0	0	0	0	0
Carbon dioxide	tons/year	0	0	0	0	0
Acetaldehyde	tons/year	1.9309E-05	1.9309E-05	8.6345E-12	0	8.637E-12
Diethyl ether	tons/year	6.1723E-07	6.1723E-07	2.3647E-12	0	2.370E-12
Water	tons/year	12405.3357	12399.958	5.3774	0	5.3775
Ethylene glycol	tons/year	106457.234	43.1823	106414.0521	43.1826	1.065E+05

Table C3. Stream results of acetaldehyde production capacity of 60,000 tons/year at 200°C

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	°C	30	30	52.49	200	200	120.89	45
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Molar Vapor Fraction		0	1	0.3023	1	1	1	0.2262
Mole Flows	kmol/hr	158.346	336.7925	1659.7817	1659.7817	1730.2223	1730.22234	1730.2223
Mass Flows	tons/year	69944.509	94265.68	678956.68	678956.68	678956.68	678956.683	678956.68
Ethanol	tons/year	69594.786	0	581767.53	581767.53	517773.1	517773.103	517773.1
Oxygen	tons/year	0	21816.541	21816.541	21816.541	36.2948	36.2948	36.2948
Nitrogen	tons/year	0	71182.794	71182.794	71182.794	71182.794	71182.7944	71182.794
Argon	tons/year	0	1209.0553	1209.0553	1209.0553	1209.0553	1209.0553	1209.0553
Carbon dioxide	tons/year	0	57.2898	57.2898	57.2898	57.2898	57.2898	57.2898
Acetaldehyde	tons/year	0	0	153.2159	153.2159	60123.5053	60123.5053	60123.505
Diethyl ether	tons/year	0	0	2.9320	2.9320	1032.5707	1032.5707	1032.5707
Water	tons/year	349.7225	0	2730.9267	2730.9267	27505.6729	27505.6729	27505.673
Ethylene glycol	tons/year	0	0	36.3967	36.3967	36.3967	36.3967	36.3967

Table C3. Stream results of acetaldehyde production capacity of 60,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	10	10	10	10.08	31.06	31.06	31.12
Pressure	bar	1.01325	1.01325	1.01325	2.34	2	2	2.54
Molar Vapor Fraction		0.1607	1	0	0	1	0	0
Mole Flows	kmol/hr	1730.2223	278.1101	1452.1123	1452.1123	1.3922	137.8279	137.8279
Mass Flows	tons/year	678956.68	77515.743	601440.94	601440.94	541.1340	58777.88	58777.88
Ethanol	tons/year	517773.1	2973.3395	514799.76	514799.76	0.0143	51.4607	51.4607
Oxygen	tons/year	36.2948	36.2037	0.0911	0.0911	0.0793	0.0118	0.0118
Nitrogen	tons/year	71182.794	71078.369	104.4251	104.42506	95.5894	8.8356	8.8356
Argon	tons/year	1209.0553	1205.84	3.2153	3.2153	3.1863	0.0290	0.0290
Carbon dioxide	tons/year	57.2898	55.13754	2.1523	2.1523	1.8306	0.3217	0.3217
Acetaldehyde	tons/year	60123.505	1845.3134	58278.192	58278.192	429.636	57695.339	57695.339
Diethyl ether	tons/year	1032.5707	161.8291	870.7416	870.74156	10.3723	857.4372	857.4372
Water	tons/year	27505.673	159.7107	27345.962	27345.962	0.4257	164.4451	164.4451
Ethylene glycol	tons/year	36.3967	5.825E-05	36.3967	36.3967	5.7527E-20	5.989E-14	5.989E-14

Table C3. Stream results of acetaldehyde production capacity of 60,000 tons/year at 200°C (Cont'd)

Stream No.	**Unit**	**15**	**16**	**17**	**18**	**19**	**20**	**21**
Temperature	°C	41.52	47.20	40.66	30	100.89	96.52	78.24
Pressure	bar	2.2	2.54	2.05	2.05	2.34	2	1.01325
Molar Vapor Fraction		1	0	0.0365	0	0	0	0.0716
Mole Flows	kmol/hr	6.1735	131.6545	131.65446	131.65446	1312.8921	1164.6472	1164.6432
Mass Flows	tons/year	2830.8848	55946.995	55946.995	55946.995	542121.93	514748.264	514746.49
Ethanol	tons/year	8.992E-12	51.4607	51.4607	51.4607	514748.29	512174.506	512172.75
Oxygen	tons/year	0.0118	1.6884E-30	1.6884E-30	1.6884E-30	5.6545E-17	0	0
Nitrogen	tons/year	8.8356	8.7480E-30	8.7480E-30	8.7480E-30	8.8038E-15	0	0
Argon	tons/year	0.0290	2.41E-45	2.41E-45	2.41E-45	2.88E-15	0	0
Carbon dioxide	tons/year	0.3217	1.42E-30	1.42E-30	1.42E-30	1.92E-11	0	0
Acetaldehyde	tons/year	2307.8136	55387.525	55387.525	55387.525	153.2170	153.2169	153.2159
Diethyl ether	tons/year	513.64	343.7972	343.7972	343.7972	2.9321	2.9321	2.9320
Water	tons/year	0.2330	164.2121	164.2121	164.2121	27181.091	2381.2123	2381.2042
Ethylene glycol	tons/year	0	0	0	0	36.3967	36.3962	36.3967

Table C3. Stream results of acetaldehyde production capacity of 60,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	22	23	24	25	26
Temperature	°C	159.74	110.92	227.33	227.40	227.33
Pressure	bar	2.34	2	2.34	2.34	2.34
Molar Vapor Fraction		0	0	0	0	2.74E-09
Mole Flows	kmol/hr	503.3070	148.3890	354.918	0.144	355.062
Mass Flows	tons/year	240298.89	27460.027	212838.86	86.3652	212925.23
Ethanol	tons/year	2573.7838	2573.7822	1.5637E-03	0	1.5637E-03
Oxygen	tons/year	0	0	0	0	0
Nitrogen	tons/year	0	0	0	0	0
Argon	tons/year	0	0	0	0	0
Carbon dioxide	tons/year	0	0	0	0	0
Acetaldehyde	tons/year	3.8622E-05	3.8622E-05	1.7271E-11	0	1.7275E-11
Diethyl ether	tons/year	1.2343E-06	1.2343E-06	4.7286E-12	0	4.7426E-12
Water	tons/year	24810.634	24799.879	10.7549	0	10.7548
Ethylene glycol	tons/year	212914.47	86.3659	212828.1	86.3652	212914.47

Table C4. Stream results of acetaldehyde production capacity of 90,000 tons/year at 200°C

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	°C	30	30	52.49	200	200	120.89	45
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Molar Vapor Fraction		0	1	0.3023	1	1	1	0.2262
Mole Flows	kmol/hr	237.51	505.1887	2489.6733	2489.6733	2595.3344	2595.3344	2595.3344
Mass Flows	tons/year	104912.79	141398.51	1018435.4	1018435.4	1018435.4	1018435.4	1018435.4
Ethanol	tons/year	104388.22	0	872651.67	872651.67	776659.99	776659.99	776659.99
Oxygen	tons/year	0	32724.8084	32724.808	32724.808	54.4258	54.4258	54.4258
Nitrogen	tons/year	0	106774.184	106774.18	106774.18	106774.18	106774.18	106774.18
Argon	tons/year	0	1813.5828	1813.5828	1813.5828	1813.5828	1813.5828	1813.5828
Carbon dioxide	tons/year	0	85.9347	85.9347	85.9347	85.9347	85.9347	85.9347
Acetaldehyde	tons/year	0	0	229.8263	229.8263	90185.299	90185.299	90185.299
Diethyl ether	tons/year	0	0	4.3981	4.3981	1548.8566	1548.8566	1548.8566
Water	tons/year	524.5639	0	4096.3925	4096.3925	41258.528	41258.528	41258.528
Ethylene glycol	tons/year	0	0	54.5778	54.5778	54.5778	54.5778	54.5778

Table C4. Stream results of acetaldehyde production capacity of 90,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	10	10	10	10.08	31.06	31.06	31.11
Pressure	bar	1.01325	1.01325	1.01325	2.34	2	2	2.54
Molar Vapor Fraction		0.1607	1	0	0	1	0	0
Mole Flows	kmol/hr	2595.3344	417.1650	2178.1693	2178.1693	2.0883	206.7420	206.7420
Mass Flows	tons/year	1018435.4	116273.59	902161.79	902161.79	811.7013	88166.8613	88166.861
Ethanol	tons/year	776659.99	4460.0083	772199.98	772199.98	0.0215	77.1909	77.1909
Oxygen	tons/year	54.4258	54.2892	0.1366	0.1366	0.1189	0.0177	0.0177
Nitrogen	tons/year	106774.18	106617.55	156.6377	156.6377	143.3842	13.2534	13.2534
Argon	tons/year	1813.5828	1808.7598	4.8230	4.8230	4.7794	0.0435	0.0435
Carbon dioxide	tons/year	85.9347	82.7063	3.2284	3.2284	2.7459	0.4826	0.4826
Acetaldehyde	tons/year	90185.299	2767.9696	87417.329	87417.329	644.4543	86543.05	86543.05
Diethyl ether	tons/year	1548.8566	242.7436	1306.113	1306.113	15.5585	1286.1565	1286.1565
Water	tons/year	41258.528	239.56596	41018.962	41018.962	0.6386	246.6668	246.6668
Ethylene glycol	tons/year	54.5778	8.735E-05	54.5777	54.5777	8.6260E-20	8.9804E-14	8.98E-14

Table C4. Stream results of acetaldehyde production capacity of 90,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	41.52	47.20	40.66	30	100.89	96.52	78.24
Pressure	bar	2.2	2.54	2.05	2.05	2.34	2	1.01325
Molar Vapor Fraction		1	0	0.0365	0	0	0	0.0716
Mole Flows	kmol/hr	9.2602	197.4818	197.4818	197.4818	1969.339	1746.9716	1746.9746
Mass Flows	tons/year	4246.3281	83920.5332	83920.53	83920.53	813183.23	772122.75	772124.08
Ethanol	tons/year	1.349E-11	77.1909	77.1909	77.1909	772122.77	768262.12	768263.45
Oxygen	tons/year	0.0177	2.532E-30	2.532E-30	2.532E-30	8.479E-17	0	0
Nitrogen	tons/year	13.2534	1.312E-29	1.312E-29	1.312E-29	1.321E-14	0	0
Argon	tons/year	0.0435	3.620E-45	3.620E-45	3.620E-45	4.324E-15	0	0
Carbon dioxide	tons/year	0.4826	2.123E-30	2.123E-30	2.123E-30	2.887E-11	0	0
Acetaldehyde	tons/year	3461.722	83081.3278	83081.328	83081.328	229.8254	229.8254	229.8263
Diethyl ether	tons/year	770.4593	515.6972	515.6972	515.6972	4.3981	4.3981	4.3981
Water	tons/year	0.3495	246.3173	246.3173	246.3173	40771.656	3571.8235	3571.8286
Ethylene glycol	tons/year	0	0	0	0	54.5777	54.5793	54.5778

Table C4. Stream results of acetaldehyde production capacity of 90,000 tons/year at 200°C (Cont'd)

Stream No.	Unit	22	23	24	25	26
Temperature	°C	159.74	110.92	227.33	227.40	227.33
Pressure	bar	2.34	2	2.34	2.34	2.34
Molar Vapor Fraction		0	0	0	0	4.21E-09
Mole Flows	kmol/hr	754.9605	222.5835	532.377	0.216	532.593
Mass Flows	tons/year	360448.31	41190.021	319258.29	129.54788	319387.836
Ethanol	tons/year	3860.6478	3860.6455	2.346E-03	0	2.346E-03
Oxygen	tons/year	0	0	0	0	0
Nitrogen	tons/year	0	0	0	0	0
Argon	tons/year	0	0	0	0	0
Carbon dioxide	tons/year	0	0	0	0	0
Acetaldehyde	tons/year	5.792E-05	5.792E-05	2.590E-11	0	2.592E-11
Diethyl ether	tons/year	1.852E-06	1.852E-06	7.096E-12	0	7.110E-12
Water	tons/year	37215.966	37199.834	16.1322	0	16.1331
Ethylene glycol	tons/year	319371.7	129.5419	319242.16	129.5479	319371.7

Table C5. Stream results of acetaldehyde production capacity of 12,000 tons/year at 300°C

Stream No,	**Unit**	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Temperature	°C	30	30	8.17	300	300	90	429.05
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	10
Molar Vapor Fraction		0	1	0.8350	1	1	1	1
Mole Flows	kmol/hr	56.4773	243.96922	300.4465	300.4465	347.0124	347.0124	347.0124
Mass Flows	tons/year	24947.13	68285.14	93232.27	93232.27	93232.27	93232.27	93232.27
Ethanol	tons/year	24822.394	0	24822.394	24822.394	496.4479	496.4479	496.4479
Oxygen	tons/year	0	15803.689	15803.689	15803.689	24.5173	24.5173	24.5173
Nitrogen	tons/year	0	51564.123	51564.123	51564.123	51564.123	51564.123	51564.123
Argon	tons/year	0	875.82786	875.8279	875.8279	875.8279	875.8279	875.8279
Carbon dioxide	tons/year	0	41.500196	41.5002	41.5002	6325.4076	6325.4076	6325.4076
Acetaldehyde	tons/year	0	0	0	0	11996.286	11996.286	11996.286
Carbon monoxide	tons/year	0	0	0	0	3999.4447	3999.4447	3999.4447
Ethylene	tons/year	0	0	0	0	2794.8757	2794.8757	2794.8757
Diethyl ether	tons/year	0	0	0	0	493.2343	493.2343	493.2343
Water	tons/year	124.7357	0	124.7357	124.7357	14662.106	14662.106	14662.106

Table C5. Stream results of acetaldehyde production capacity of 12,000 tons/year at 300°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	139.4	45	10	10	10	9.96	34.48
Pressure	bar	10	10	10	10	10	2.34	2
Molar Vapor Fraction		1	0.7426	0.6928	1	0	3.1346E-04	1
Mole Flows	kmol/hr	347.0124	347.0124	347.0124	240.4020	106.6103	106.6103	0.6484
Mass Flows	tons/year	93232.27	93232.27	93232.27	68899.282	24332.988	24332.988	273.8801
Ethanol	tons/year	496.4479	496.4479	496.4479	4.3155	492.1324	492.1324	1.916E-06
Oxygen	tons/year	24.5173	24.5173	24.5173	24.5126	4.635E-03	4.635E-03	4.401E-03
Nitrogen	tons/year	51564.123	51564.123	51564.1226	51559.268	4.8545	4.8545	4.6982
Argon	tons/year	875.8279	875.8279	875.8279	875.6519	0.1759	0.1759	0.1757
Carbon dioxide	tons/year	6325.4076	6325.4076	6325.4076	6290.0601	35.3475	35.3475	34.2413
Acetaldehyde	tons/year	11996.286	11996.286	11996.286	2974.8428	9021.4432	9021.4432	225.6494
Carbon monoxide	tons/year	3999.4447	3999.4447	3999.4447	3998.8878	0.5569	0.5569	0.5330
Ethylene	tons/year	2794.8757	2794.8757	2794.8757	2792.7902	2.0855	2.0855	2.0756
Diethyl ether	tons/year	493.2343	493.2343	493.2343	336.24029	156.9940	156.9940	6.2188
Water	tons/year	14662.106	14662.106	14662.106	42.7129	14619.393	14619.393	0.2838

Table C5. Stream results of acetaldehyde production capacity of 12,000 tons/year at 300°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	34.48	119.40	34.61	45.44	50.70	40.63	30
Pressure	bar	2	2.34	2.84	2.5	2.84	2.05	2.05
Molar Vapor Fraction		0	0	0	1	0	0.0564	0
Mole Flows	kmol/hr	20.9641	84.9978	20.9641	0.9564	20.0078	20.0078	20.0078
Mass Flows	tons/year	8947.1454	15111.9622	8947.1454	444.0251	8503.1203	8503.1203	8503.1203
Ethanol	tons/year	1.757E-03	492.1306	1.757E-03	6.995E-16	1.757E-03	1.757E-03	1.757E-03
Oxygen	tons/year	2.341E-04	2.279E-19	2.341E-04	2.341E-04	4.007E-41	4.007E-41	4.007E-41
Nitrogen	tons/year	0.1563	1.592E-17	0.1563	0.1563	3.542E-41	3.542E-41	3.542E-41
Argon	tons/year	2.565E-04	1.020E-17	2.565E-04	2.565E-04	1.000E-65	1.000E-65	1.000E-65
Carbon dioxide	tons/year	1.1063	3.337E-10	1.1063	1.1063	8.346E-43	8.346E-43	8.346E-43
Acetaldehyde	tons/year	8768.8428	26.9510	8768.8428	350.7538	8418.0890	8418.0890	8418.0890
Carbon monoxide	tons/year	0.0239	8.569E-18	0.0239	0.0239	3.067E-40	3.067E-40	3.067E-40
Ethylene	tons/year	9.947E-03	2.859E-14	9.947E-03	9.947E-03	9.046E-57	9.046E-57	9.046E-57
Diethyl ether	tons/year	150.7749	0.0003	150.7749	91.8228	58.9521	58.9521	58.9521
Water	tons/year	26.2291	14592.8803	26.2291	0.1517	26.0774	26.0774	26.0774

Table C6. Stream results of acetaldehyde production capacity of 30,000 tons/year at 300°C

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	°C	30	30	8.17	300	300	90	429.05
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	10
Molar Vapor Fraction		0	1	0.8350	1	1	1	1
Mole Flows	kmol/hr	141.1933	609.9230	751.1163	751.1163	867.5308	867.5308	867.5308
Mass Flows	tons/year	62367.81	170712.84	233080.65	233080.65	233080.65	233080.65	233080.65
Ethanol	tons/year	62055.971	0	62055.971	62055.971	1241.1194	1241.1194	1241.1194
Oxygen	tons/year	0	39509.221	39509.221	39509.221	61.3004	61.3004	61.3004
Nitrogen	tons/year	0	128910.3	128910.3	128910.3	128910.3	128910.3	128910.3
Argon	tons/year	0	2189.5695	2189.5695	2189.5695	2189.5695	2189.5695	2189.5695
Carbon dioxide	tons/year	0	103.7505	103.7505	103.7505	15813.5152	15813.5152	15813.5152
Acetaldehyde	tons/year	0	0	0	0	29990.708	29990.708	29990.708
Carbon monoxide	tons/year	0	0	0	0	9998.6093	9998.6093	9998.6093
Ethylene	tons/year	0	0	0	0	6987.1876	6987.1876	6987.1876
Diethyl ether	tons/year	0	0	0	0	1233.0855	1233.0855	1233.0855
Water	tons/year	311.8391	0	311.8391	311.8391	36655.256	36655.256	36655.256

Table C6. Stream results of acetaldehyde production capacity of 30,000 tons/year at 300°C (Cont'd)

Stream No.	**Unit**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Temperature	°C	139.4	45	10	10	10	9.96	34.48
Pressure	bar	10	10	10	10	10	2.34	2
Molar Vapor Fraction		1	0.7426	0.6928	1	0	3.135E-04	1
Mole Flows	kmol/hr	867.5308	867.5308	867.5308	601.0050	266.5258	266.5258	1.6209
Mass Flows	tons/year	233080.65	233080.65	233080.65	172248.1966	60832.4534	60832.4534	684.6998
Ethanol	tons/year	1241.1194	1241.1194	1241.1194	10.7888	1230.3307	1230.3307	4.789E-06
Oxygen	tons/year	61.3004	61.3004	61.3004	61.2888	0.0116	0.0116	0.0110
Nitrogen	tons/year	128910.299	128910.299	128910.299	128898.163	12.1362	12.1362	11.7455
Argon	tons/year	2189.5695	2189.5695	2189.5695	2189.1297	0.4398	0.4398	0.4392
Carbon dioxide	tons/year	15813.5152	15813.5152	15813.5152	15725.1464	88.3688	88.3688	85.6031
Acetaldehyde	tons/year	29990.7079	29990.7079	29990.7079	7437.1065	22553.6014	22553.6014	564.1231
Carbon monoxide	tons/year	9998.6093	9998.6093	9998.6093	9997.2171	1.3922	1.3922	1.3325
Ethylene	tons/year	6987.1876	6987.1876	6987.1876	6981.9738	5.2138	5.2138	5.1889
Diethyl ether	tons/year	1233.0855	1233.0855	1233.0855	840.6006	392.4849	392.4849	15.5470
Water	tons/year	36655.2563	36655.2563	36655.2563	106.7823	36548.4740	36548.4740	0.7094

Table C6. Stream results of acetaldehyde production capacity of 30,000 tons/year at 300°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	34.48	119.40	34.61	45.44	50.70	40.63	30
Pressure	bar	2	2.34	2.84	2.5	2.84	2.05	2.05
Molar Vapor Fraction		0	0	0	1	0	0.0564	0
Mole Flows	kmol/hr	52.4103	212.4946	52.4103	2.3909	50.0194	50.0194	50.0194
Mass Flows	tons/year	22367.8512	37779.9024	22367.8512	1110.0567	21257.7945	21257.7945	21257.7945
Ethanol	tons/year	4.390E-03	1230.3263	4.390E-03	1.75E-15	4.390E-03	4.390E-03	4.390E-03
Oxygen	tons/year	5.854E-04	5.696E-19	5.854E-04	5.854E-04	1.003E-40	1.003E-40	1.003E-40
Nitrogen	tons/year	0.3907	3.979E-17	0.3907	0.3907	8.865E-41	8.865E-41	8.865E-41
Argon	tons/year	6.414E-04	2.550E-17	6.414E-04	6.414E-04	2.502E-65	2.502E-65	2.502E-65
Carbon dioxide	tons/year	2.7657	8.339E-10	2.7657	2.7657	2.087E-42	2.087E-42	2.087E-42
Acetaldehyde	tons/year	21922.1006	67.3778	21922.1006	876.8840	21045.2165	21045.2165	21045.2165
Carbon monoxide	tons/year	0.0597	2.142E-17	0.0597	0.0597	7.676E-40	7.676E-40	7.676E-40
Ethylene	tons/year	0.0249	7.146E-14	0.0249	0.0249	2.262E-56	2.262E-56	2.262E-56
Diethyl ether	tons/year	376.9372	6.717E-04	376.9372	229.5514	147.3858	147.3858	147.3858
Water	tons/year	65.5669	36482.198	65.5669	0.3792	65.1878	65.1878	65.1878

Table C7. Stream results of acetaldehyde production capacity of 60,000 tons/year at 300°C

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	°C	30	30	8.17	300	300	90	429.05
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	10
Molar Vapor Fraction		0	1	0.8350	1	1	1	1
Mole Flows	kmol/hr	282.3865	1219.846	1502.2326	1502.2326	1735.0616	1735.06163	1735.0616
Mass Flows	tons/year	124735.63	341425.68	466161.31	466161.31	466161.31	466161.31	466161.31
Ethanol	tons/year	124111.95	0	124111.95	124111.95	2482.239	2482.239	2482.239
Oxygen	tons/year	0	79018.442	79018.442	79018.442	122.5944	122.5944	122.5944
Nitrogen	tons/year	0	257820.6	257820.6	257820.6	257820.6	257820.598	257820.6
Argon	tons/year	0	4379.139	4379.139	4379.139	4379.139	4379.13903	4379.139
Carbon dioxide	tons/year	0	207.501	207.501	207.501	31627.033	31627.033	31627.033
Acetaldehyde	tons/year	0	0	0	0	59981.421	59981.4206	59981.421
Carbon monoxide	tons/year	0	0	0	0	19997.22	19997.2202	19997.22
Ethylene	tons/year	0	0	0	0	13974.376	13974.3762	13974.376
Diethyl ether	tons/year	0	0	0	0	2466.1712	2466.1712	2466.1712
Water	tons/year	623.6782	0	623.6782	623.6782	73310.518	73310.5185	73310.518

Table C7. Stream results of acetaldehyde production capacity of 60,000 tons/year at 300°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	139.4	45	10	10	10	9.96	34.48
Pressure	bar	10	10	10	10	10	2.34	2
Molar Vapor Fraction		1	0.7426	0.6928	1	0	3.135E-04	1
Mole Flows	kmol/hr	1735.0616	1735.0616	1735.0616	1202.0101	533.0516	533.05156	3.2419
Mass Flows	tons/year	466161.31	466161.31	466161.31	344496.39	121664.92	121664.92	1369.3957
Ethanol	tons/year	2482.239	2482.239	2482.239	21.5775	2460.6615	2460.6615	9.56E-06
Oxygen	tons/year	122.5944	122.5944	122.5944	122.5713	0.0232	0.0232	0.0220
Nitrogen	tons/year	257820.6	257820.6	257820.6	257796.33	24.2725	24.2725	23.4908
Argon	tons/year	4379.139	4379.139	4379.139	4378.2594	0.8797	0.8797	0.8784
Carbon dioxide	tons/year	31627.033	31627.033	31627.033	31450.295	176.7376	176.7376	171.2064
Acetaldehyde	tons/year	59981.421	59981.421	59981.421	14874.213	45107.208	45107.208	1128.2433
Carbon monoxide	tons/year	19997.22	19997.22	19997.22	19994.436	2.7843	2.7843	2.6649
Ethylene	tons/year	13974.376	13974.376	13974.376	13963.949	10.4276	10.4276	10.3779
Diethyl ether	tons/year	2466.1712	2466.1712	2466.1712	1681.2012	784.970	784.970	31.0940
Water	tons/year	73310.518	73310.518	73310.518	213.5646	73096.954	73096.954	1.4181

Table C7. Stream results of acetaldehyde production capacity of 60,000 tons/year at 300°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	34.48	119.40	34.59	45.44	50.70	40.63	30
Pressure	bar	2	2.34	2.84	2.5	2.84	2.05	2.05
Molar Vapor Fraction		0	0	0	1	0	0.0564	0
Mole Flows	kmol/hr	104.8201	424.98955	104.82014	4.7817	100.0384	100.0384	100.0384
Mass Flows	tons/year	44735.638	75559.884	44735.638	2220.0444	42515.593	42515.5935	42515.593
Ethanol	tons/year	8.762E-03	2460.6527	8.762E-03	3.49E-15	8.762E-03	8.762E-03	8.762E-03
Oxygen	tons/year	1.171E-03	1.137E-18	1.171E-03	1.171E-03	2.020E-40	2.020E-40	2.020E-40
Nitrogen	tons/year	0.7817	7.944E-17	0.7817	0.7817	1.786E-40	1.786E-40	1.786E-40
Argon	tons/year	1.28E-03	5.091E-17	1.283E-03	1.283E-03	5.012E-65	5.012E-65	5.012E-65
Carbon dioxide	tons/year	5.5313	1.665E-09	5.5313	5.5313	4.181E-42	4.181E-42	4.181E-42
Acetaldehyde	tons/year	43844.206	134.7585	43844.206	1753.7683	42090.437	42090.4374	42090.437
Carbon monoxide	tons/year	0.1194	4.275E-17	0.1194	0.1194	1.546E-39	1.546E-39	1.546E-39
Ethylene	tons/year	0.0497	1.427E-13	0.0497	0.0497	4.531E-56	4.531E-56	4.531E-56
Diethyl ether	tons/year	753.8746	1.344E-03	753.87462	459.0333	294.8413	294.841295	294.8413
Water	tons/year	131.0642	72964.472	131.0642	0.7582	130.3060	130.3060	130.3060

Table C8. Stream results of acetaldehyde production capacity of 90,000 tons/year at 300°C

Stream No.	Unit	1	2	3	4	5	6	7
Temperature	°C	30	30	8.17	300	300	90	429.05
Pressure	bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	10
Molar Vapor Fraction		0	1	0.8350	1	1	1	1
Mole Flows	kmol/hr	423.5798	1829.7690	2253.3488	2253.3488	2602.5924	2602.5924	2602.5924
Mass Flows	tons/year	187103.44	512138.52	699241.96	699241.96	699241.96	699241.96	699241.96
Ethanol	tons/year	186167.92	0	186167.92	186167.923	3723.3585	3723.3585	3723.3585
Oxygen	tons/year	0	118527.66	118527.66	118527.663	183.8948	183.8948	183.8948
Nitrogen	tons/year	0	386730.9	386730.9	386730.897	386730.897	386730.9	386730.9
Argon	tons/year	0	6568.7085	6568.7085	6568.7085	6568.7085	6568.7085	6568.7085
Carbon dioxide	tons/year	0	311.2515	311.2515	311.2515	47440.5482	47440.548	47440.548
Acetaldehyde	tons/year	0	0	0	0	89972.1285	89972.128	89972.128
Carbon monoxide	tons/year	0	0	0	0	29995.8294	29995.829	29995.829
Ethylene	tons/year	0	0	0	0	20961.5638	20961.564	20961.564
Diethyl ether	tons/year	0	0	0	0	3699.2567	3699.2567	3699.2567
Water	tons/year	935.5172	0	935.5172	935.5172	109965.77	109965.77	109965.77

Table C8. Stream results of acetaldehyde production capacity of 90,000 tons/year at 300°C (Cont'd)

Stream No.	Unit	8	9	10	11	12	13	14
Temperature	°C	139.4	45	10	10	10	9.96	34.48
Pressure	bar	10	10	10	10	10	2.34	2
Molar Vapor Fraction		1	0.7426	0.6928	1	0	3.135E-04	1
Mole Flows	kmol/hr	2602.5924	2602.5924	2602.5924	1803.0151	799.5773	799.577303	4.8628
Mass Flows	tons/year	699241.96	699241.96	699241.96	516744.59	182497.37	182497.371	2054.1034
Ethanol	tons/year	3723.3585	3723.3585	3723.3585	32.3663	3690.9922	3690.99217	1.438E-05
Oxygen	tons/year	183.8948	183.8948	183.8948	183.8600	0.0348	0.0348	0.0330
Nitrogen	tons/year	386730.9	386730.9	386730.9	386694.49	36.4087	36.4087	35.2369
Argon	tons/year	6568.7085	6568.7085	6568.7085	6567.389	1.3195	1.3195	1.3176
Carbon dioxide	tons/year	47440.548	47440.548	47440.548	47175.442	265.1064	265.1064	256.8093
Acetaldehyde	tons/year	89972.128	89972.128	89972.128	22311.32	67660.809	67660.809	1692.3722
Carbon monoxide	tons/year	29995.829	29995.829	29995.829	29991.653	4.1765	4.1765	3.9975
Ethylene	tons/year	20961.564	20961.564	20961.564	20945.922	15.641387	15.6414	15.5668
Diethyl ether	tons/year	3699.2567	3699.2567	3699.2567	2521.8018	1177.4548	1177.4548	46.6412
Water	tons/year	109965.77	109965.77	109965.77	320.3469	109645.43	109645.4278	2.1289

Table C8. Stream results of acetaldehyde production capacity of 90,000 tons/year at 300°C (Cont'd)

Stream No.	Unit	15	16	17	18	19	20	21
Temperature	°C	34.48	119.40	34.57	45.44	50.70	40.63	30
Pressure	bar	2	2.34	2.84	2.5	2.84	2.05	2.05
Molar Vapor Fraction		0	0	0	1	0	0.0564	0
Mole Flows	kmol/hr	157.2312	637.4833	157.2312	7.1728	150.0584	150.0584	150.0584
Mass Flows	tons/year	67103.624	113339.64	67103.624	3330.2359	63773.388	63773.388	63773.388
Ethanol	tons/year	0.0132	3690.9790	0.0132	5.250E-15	0.0132	0.0132	0.0132
Oxygen	tons/year	1.756E-03	1.711E-18	1.756E-03	1.756E-03	2.996E-40	2.996E-40	2.996E-40
Nitrogen	tons/year	1.1718	1.195E-16	1.1718	1.1718	2.648E-40	2.648E-40	2.648E-40
Argon	tons/year	0.0019241	7.660E-17	1.924E-03	1.924E-03	7.498E-65	7.498E-65	7.498E-65
Carbon dioxide	tons/year	8.2971	2.505E-09	8.2971	8.2971	6.254E-42	6.254E-42	6.254E-42
Acetaldehyde	tons/year	65766.306	202.13047	65766.306	2630.65235	63135.6539	63135.654	63135.654
Carbon monoxide	tons/year	0.1790	6.432E-17	0.1790	0.1790	2.293E-39	2.293E-39	2.293E-39
Ethylene	tons/year	0.0746	2.146E-13	0.0746	0.0746	6.779E-56	6.779E-56	6.779E-56
Diethyl ether	tons/year	1130.8116	2.014E-03	1130.8116	688.7197	442.0919	442.0919	442.0919
Water	tons/year	196.7666	109446.53	196.7666	1.1376	195.6290	195.6290	195.6290

APPENDIX D UTILITIES SPECIFICATIONS

Table D1. Utilities specification for acetaldehyde production at 200°C

Name	Utility type	Temperature (°C)	
		Inlet	Outlet
CW	Water	35	50
CHILLED	Water	4	10
LPS	Steam	125	124
MPS	Steam	175	174
HPS	Steam	250	249
FIREHEAT	Gas	1,000	400
BFW	Water	110.89	110.89
GC	Refrigeration	0	10

Table D2. Utilities specification for acetaldehyde production at 300°C

Name	Utility type	Temperature (°C)	
		Inlet	Outlet
CW	Water	35	50
CHILLED	Water	4	10
LPS	Steam	125	124
MPS	Steam	175	174
HPS	Steam	250	249
FIREHEAT	Gas	1,000	400
BFW	Water	129.40	129.40
GC	Refrigeration	0	10

APPENDIX E EQUIPMENT SPECIFICATIONS

E.1 Acetaldehyde production at 200°C

E.1.1 Heat exchanger specifications

Table E1. Size of heat exchangers

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kg/hr)	Heat duty (kW)	Area (m^2)
12,000	H101	BFW	888.15	545.20	301.48
	H102	CW	205,361.60	3,570.61	509.81
	H103	GC	66,028.80	646.37	55.75
	H104	CHILLED	2,421.96	16.93	1.57
30,000	H101	BFW	2,220.38	1,362.98	753.69
	H102	CW	513,400.31	8,926.47	1,274.51
	H103	GC	165,071.71	1,615.91	139.37
	H104	CHILLED	6,054.86	42.32	3.92
60,000	H101	BFW	4,440.77	2,725.95	1,507.38
	H102	CW	1.027E+06	17,852.91	2,549.01
	H103	GC	330,142.39	3,231.82	278.74
	H104	CHILLED	12,109.70	84.64	7.83
90,000	H101	BFW	6,661.15	4,088.93	2,261.07
	H102	CW	1.54E+06	26,779.38	3,823.52
	H103	GC	495,215.65	4,847.74	418.11
	H104	CHILLED	18,164.56	126.96	11.75
120,000	H101	BFW	8,881.53	5,451.91	3,014.76
	H102	CW	2.054E+06	35,705.87	5,098.03
	H103	GC	660,285.81	6,463.65	557.48
	H104	CHILLED	24,219.43	169.28	15.66

E.1.2 Distillation column specifications

Table E2. Distillation column specifications

Unit code	Condenser	Reboiler	Reflux ratio	Number of stages	Feed location
D101	Partial-vap-liq	Kettle	3.93	11	6
D102	Partial-vapor	Kettle	26.90	19	9
D103	Total	Kettle	1.01	34	26
D104	Total	Kettle	1	9	5

Table E3. Size of distillation columns

Acetaldehyde production capacity (tons/year)	Unit code	Unit name	Utility	Utility usage (kg/hr)	Heat duty (kW)
12,000	D101	Condenser	CHILLED	142,108.81	-993.27
		Reboiler	LPS	3,386.62	2,061.96
	D102	Condenser	CHILLED	32,252.41	-225.43
		Reboiler	LPS	410.70	250.06
	D103	Condenser	CW	282,923.04	-4,919.17
		Reboiler	MPS	8,229.35	4,651.30
	D104	Condenser	CW	38,392.30	-667.52
		Reboiler	HPS	1,865.76	891.07
30,000	D101	Condenser	CHILLED	355,235.49	-2,482.93
		Reboiler	LPS	8,467.04	5,155.20
	D102	Condenser	CHILLED	80,629.64	-563.56
		Reboiler	LPS	1,026.74	625.14
	D103	Condenser	CW	707,320.72	-12,298.15
		Reboiler	MPS	20,573.82	11,628.50
	D104	Condenser	CW	95,970.57	-1,668.64
		Reboiler	HPS	4,664.04	2,227.50

Table E3. Size of distillation columns (Cont'd)

Acetaldehyde production capacity (tons/year)	Unit code	Unit name	Utility	Utility usage (kg/hr)	Heat duty (kW)
60,000	D101	Condenser	CHILLED	710,437.25	-4,965.62
		Reboiler	LPS	16,934.54	10,310.69
	D102	Condenser	CHILLED	161,251.55	-1,127.07
		Reboiler	LPS	2,053.55	1,250.32
	D103	Condenser	CW	1.415E+06	-24,595.91
		Reboiler	MPS	41,146.91	23,256.60
	D104	Condenser	CW	191,940.90	-3,337.27
		Reboiler	HPS	9,328.08	4,454.99
90,000	D101	Condenser	CHILLED	1.066E+06	-7,448.29
		Reboiler	LPS	25,402.16	15,466.24
	D102	Condenser	CHILLED	241,870.66	-1,690.56
		Reboiler	LPS	3,080.35	1,875.49
	D103	Condenser	CW	2.12E+06	-36,894.68
		Reboiler	MPS	61,721.86	34,885.74
	D104	Condenser	CW	287,911.33	-5,005.90
		Reboiler	HPS	13,992.11	6,682.49
120,000	D101	Condenser	CHILLED	1.42E+06	-9,930.95
		Reboiler	LPS	33,869.83	20,621.82
	D102	Condenser	CHILLED	322,488.87	-2,254.04
		Reboiler	LPS	4,107.15	2,500.66
	D103	Condenser	CW	2.83E+06	-49,191.67
		Reboiler	MPS	82,293.55	46,513.03
	D104	Condenser	CW	383,879.16	-6.674.49
		Reboiler	HPS	18,656.07	8,909.95

E.1.3 Furnace specifications

Table E4. Size of furnace

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kg/hr)	Heat duty (kW)
12,000	FH101	FIREHEAT	21,549.47	3,591.58
30,000	FH101	FIREHEAT	53,873.28	8,978.88
60,000	FH101	FIREHEAT	107,746.57	17,957.76
90,000	FH101	FIREHEAT	161,619.39	26,936.56
120,000	FH101	FIREHEAT	215,493.19	35,915.53

E.1.4 Pump specifications

Table E5. Size of pumps

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kW)	Electrical duty (kW)
12,000	P101	Electricity		
	P102	Electricity		
30,000	P101	Electricity	2.33	2.33
	P102	Electricity	0.20	0.20
60,000	P101	Electricity	4.14	4.14
	P102	Electricity	0.31	0.31
90,000	P101	Electricity	5.87	5.87
	P102	Electricity	0.40	0.40
120,000	P101	Electricity	7.56	7.56
	P102	Electricity	0.49	0.49

E.2 Acetaldehyde production at 300°C

E.2.1 Heat exchanger specifications

Table E6. Size of heat exchangers

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kg/hr)	Heat duty (kW)	Area (m^2)
12,000	H201	CW	42,196.52	733.67	103.43
	H202	BFW	1,762.80	1,056.69	248.08
	H203	CW	78,696.48	1,368.29	73.04
	H204	GC	36,535.76	357.65	30.85
	H205	CHILLED	2,226.16	15.56	1.30
30,000	H201	CW	105,491.30	1,834.17	258.57
	H202	BFW	4,406.99	2,641.71	620.19
	H203	CW	196,741.15	3,420.73	182.59
	H204	GC	91,339.41	894.14	77.12
	H205	CHILLED	5,565.38	38.90	3.25
60,000	H201	CW	210,982.60	3,668.35	517.14
	H202	BFW	8,813.98	5,283.43	1,240.37
	H203	CW	393,482.34	6,841.46	365.18
	H204	GC	182,678.30	1,788.27	154.24
	H205	CHILLED	11,130.73	77.80	6.50
90,000	H201	CW	316,473.89	5,502.52	775.71
	H202	BFW	13,220.96	7,925.14	1,860.56
	H203	CW	590,223.49	10,262.19	547.78
	H204	GC	274,018.22	2,682.41	231.36
	H205	CHILLED	16,696.19	116.70	9.75

Table E6. Size of heat exchangers (Cont'd)

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kg/hr)	Heat duty (kW)	Area (m^2)
120,000	H201	CW	421,965.20	7,336.69	1,034.28
	H202	BFW	17,627.95	10,566.86	2,480.75
	H203	CW	786,964.68	13,682.92	730.37
	H204	GC	365,357.63	3,576.54	308.47
	H205	CHILLED	22,261.55	155.60	13.00

E.2.2 Distillation column specifications

Table E7. Distillation column specifications

Unit code	Condenser	Reboiler	Reflux ratio	Number of stages	Feed location
D201	Partial-vap-liq	Kettle	3.26	8	5
D202	Partial-vapor	Kettle	30.52	23	9

Table E8. Size of distillation columns

Acetaldehyde production capacity (tons/year)	Unit code	Unit name	Utility	Utility usage (kg/hr)	Heat duty (kW)
12,000	D201	Condenser	CHILLED	93,084.33	-650.62
		Reboiler	MPS	1,704.61	963.46
	D202	Condenser	CHILLED	28,015.62	-195.82
		Reboiler	LPS	352.80	214.81
30,000	D201	Condenser	CHILLED	232,762.89	-1,626.90
		Reboiler	MPS	4,262.18	2,409.02
	D202	Condenser	CHILLED	70,035.07	-489.51
		Reboiler	LPS	881.96	536.98

Table E8. Size of distillation columns (Cont'd)

Acetaldehyde production capacity (tons/year)	Unit code	Unit name	Utility	Utility usage (kg/hr)	Heat duty (kW)
60,000	D201	Condenser	CHILLED	466,156.53	-3,258.21
		Reboiler	MPS	8,532.16	4,822.45
	D202	Condenser	CHILLED	140,016.62	-978.65
		Reboiler	LPS	1,763.41	1,073.66
90,000	D201	Condenser	CHILLED	697,694.40	-4,876.55
		Reboiler	MPS	12,779.17	7,222.90
	D202	Condenser	CHILLED	210,126.91	-1,468.69
		Reboiler	LPS	2,646.45	1,611.30
120,000	D201	Condenser	CHILLED	930,783.41	-6,505.73
		Reboiler	MPS	17,045.38	9,634.20
	D202	Condenser	CHILLED	280,123.69	-1,957.93
		Reboiler	LPS	3,528.18	2,148.15

E.2.3 Furnace specifications

Table E9. Size of furnace

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kg/hr)	Heat duty (kW)
12,000	FH201	FIREHEAT	9,413.80	1,568.97
30,000	FH201	FIREHEAT	23,534.50	3,922.42
60,000	FH201	FIREHEAT	47,069.00	7,844.83
90,000	FH201	FIREHEAT	70,603.49	11,767.25
120,000	FH201	FIREHEAT	94,137.99	15,689.67

E.2.4 Compressor specifications

Table E10. Size of compressor

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kW)	Electrical duty (kW)
12,000	C201	Electricity	1,222.28	1,222.28
30,000	C201	Electricity	3,055.71	3,055.71
60,000	C201	Electricity	6,111.42	6,111.42
90,000	C201	Electricity	9,167.14	9,167.14
120,000	C201	Electricity	12,222.85	12,222.85

E.2.5 Pump specifications

Table E11. Size of pump

Acetaldehyde production capacity (tons/year)	Unit code	Utility	Utility usage (kW)	Electrical duty (kW)
12,000	P201	Electricity	0.10	0.10
30,000	P201	Electricity	0.24	0.24
60,000	P201	Electricity	0.41	0.41
90,000	P201	Electricity	0.52	0.52
120,000	P201	Electricity	0.63	0.63

APPENDIX F NET CO_2 EMISSIONS

F.1 Net CO_2 emissions for acetaldehyde production at 200°C

Table F1. Indirect CO_2 emissions in the unit of kilogram per hour (kg/hr)

Unit code	Acetaldehyde production capacity					Unit
	12,000	**30,000**	**60,000**	**90,000**	**120,000**	tons/year
FH101	850.16	2,125.39	4,250.79	6,376.16	8,501.58	kg/hr
P101	0.40	0.81	1.44	2.04	2.62	kg/hr
P102	0.03	0.07	0.11	0.14	0.17	kg/hr
D101	488.09	1,220.29	2,440.65	3,661.02	4,881.40	kg/hr
D102	59.19	147.98	295.96	443.95	591.93	kg/hr
D103	1,101.01	2,752.59	5,505.08	8,257.81	11,010.10	kg/hr
D104	210.93	527.27	1,054.54	1,581.81	2,109.08	kg/hr
Net CO_2 emission	**2,709.81**	**6,774.40**	**13,548.57**	**20,322.92**	**27,096.89**	**kg/hr**

F.2 Net CO_2 emissions for acetaldehyde production at 300°C

Table F2. Indirect CO_2 emissions in the unit of kilogram per hour (kg/hr)

Unit code	Acetaldehyde production capacity					Unit
	12,000	**30,000**	**60,000**	**90,000**	**120,000**	tons/year
FH201	371.39	928.48	1,856.95	2,785.43	3,713.91	kg/hr
C201	424.01	1,060.04	2,120.07	3,180.11	4,240.14	kg/hr
P201	0.03	0.08	0.14	0.18	0.22	kg/hr
D201	228.06	570.24	1,141.52	1,709.74	2,280.51	kg/hr
D202	50.85	127.11	254.15	381.41	508.49	kg/hr
Net CO_2 emission	**1,074.35**	**2,685.95**	**5,372.83**	**8,056.87**	**10,743.27**	**kg/hr**

APPENDIX G ECONOMIC ANALYSIS RESULTS

G.1 Acetaldehyde production at 200°C

Table G1. Economic analysis results of 12,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.519231
DT (Duration of EPC Phase and Startup)	Period	0.903846
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	1.08E+07
RAWT (Total Raw Material Cost)	Cost/period	7.85E+06
PRODT (Total Product Sales)	Cost/period	2.91E+07
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	921307
UTILT (Total Utilities Cost)	Cost/period	3.30E+06
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1

Table G1. Economic analysis results of 12,000 tons/year (Cont'd)

ITEM	UNITS	
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.230769
OP (Total Operating Labor Cost)	Cost/period	832770
MT (Total Maintenance Cost)	Cost/period	88536.6

Table G1. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	2935500	11917200	10809200	11349700	11349700	567484	6837030	3907980	412381	43843
2	32055600		10809200		11349700		14691500	8413100	883486	93929
3	33658400		10809200		11349700		15177700	8707550	909990	96746
4	35341300		10809200		11349700		15680100	9012320	937290	99649
5	37108400		10809200		11349700		16199100	9327750	965409	102638
6	38963800		10809200		11349700		16735500	9654220	994371	105717
7	40912000		10809200		11349700		17289700	9992120	1024200	108889
8	42957600		10809200		11349700		17862300	10341800	1054930	112156
9	45105500		10809200		11349700		18454000	10703800	1086580	115520
10	47360800		10809200		11349700		19065500	11078400	1119170	118986

Table G1. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	49728800		10809200		11349700		19697200	11466200	1152750	122555
12	52215300		10809200		11349700		20350100	11867500	1187330	126232
13	54826000		10809200		11349700		21024700	12282900	1222950	130019
14	57567300		10809200		11349700		21721700	12712800	1259640	133920
15	60445700		10809200		11349700		22442000	13157700	1297430	137937
16	63468000		10809200		11349700		23186400	13618200	1336350	142075
17	66641400		10809200		11349700		23955500	14094900	1376440	146338
18	69973400		10809200		11349700		24750300	14588200	1417740	150728
19	73472100		10809200		11349700		25571500	15098800	1460270	155249
20	77145700		10809200		11349700		26420200	15627200	1504080	159907

Table G1. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	1635170	103095	228112	6330580	506446	-15818700	864737	-16683400	0	-16683400
2	3503190	220871	488707	13603300	1088260	17364100	864737	16499400	6599750	9899620
3	3608280	227498	503368	14053400	1124280	18480700	864737	17616000	7046390	10569600
4	3716530	234322	518469	14518600	1161490	19661300	864737	18796500	7518620	11277900
5	3828030	241352	534023	14999200	1199940	20909300	864737	20044500	8017820	12026700
6	3942870	248593	550044	15495800	1239670	22228400	864737	21363600	8545450	12818200
7	4061150	256051	566545	16009000	1280720	23622300	864737	22757600	9103040	13654600
8	4182990	263732	583542	16539200	1323140	25095300	864737	24230600	9692230	14538300
9	4308480	271644	601048	17087100	1366970	26651500	864737	25786700	10314700	15472000
10	4437730	279793	619080	17653200	1412260	28295300	864737	27430600	10972200	16458400

Table G1. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	4570860	288187	637652	18238200	1459060	30031600		30031600	12012600	18018900
12	4707990	296833	656781	18842700	1507410	31865200		31865200	12746100	19119100
13	4849230	305738	676485	19467300	1557380	33801400		33801400	13520500	20280800
14	4994710	314910	696779	20112700	1609020	35845600		35845600	14338200	21507400
15	5144550	324357	717683	20779700	1662370	38003700		38003700	15201500	22802200
16	5298880	334088	739213	21468800	1717510	40281600		40281600	16112700	24169000
17	5457850	344110	761390	22181000	1774480	42685900		42685900	17074400	25611500
18	5621590	354434	784231	22916900	1833350	45223200		45223200	18089300	27133900
19	5790230	365067	807758	23677400	1894190	47900600		47900600	19160200	28740300
20	5963940	376019	831991	24463200	1957050	50725500		50725500	20290200	30435300

Table G1. Economic analysis results of 12,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-15818700	18754200	-15818700	-13182200	-13182200
2	10764400	14691500	10764400	7475250	-5706990
3	11434300	15177700	11434300	6617080	910098
4	12142700	15680100	12142700	5855840	6765930
5	12891500	16199100	12891500	5180790	11946700
6	13682900	16735500	13682900	4582380	16529100
7	14519300	17289700	14519300	4052070	20581200
8	15403100	17862300	15403100	3582260	24163400
9	16336800	18454000	16336800	3166180	27329600
10	17323100	19065500	20025400	2797780	30563800

Table G1. Economic analysis results of 12,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	18018900	19697200		2425130	
12	19119100	20350100		2144340	
13	20280800	21024700		1895520	
14	21507400	21721700		1675130	
15	22802200	22442000		1479990	
16	24169000	23186400		1307250	
17	25611500	23955500		1154400	
18	27133900	24750300		1019180	
19	28740300	25571500		899598	
20	30435300	26420200		793876	

Table G2. Economic analysis results of 30,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.538462
DT (Duration of EPC Phase and Startup)	Period	0.923077
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	1.31E+07
RAWT (Total Raw Material Cost)	Cost/period	1.96E+07
PRODT (Total Product Sales)	Cost/period	7.27E+07
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	977409
UTILT (Total Utilities Cost)	Cost/period	8.21E+06
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G2. Economic analysis results of 30,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.25
OP (Total Operating Labor Cost)	Cost/period	832770
MT (Total Maintenance Cost)	Cost/period	144639

Table G2. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	5870950	14440200	13097700	13752600	13752600	687629	15205100	9378030	395886	68759
2	80138500		13097700		13752600		34042500	21030200	883486	153448
3	84145500		13097700		13752600		35177300	21766300	909990	158051
4	88352700		13097700		13752600		36350200	22528100	937290	162792
5	92770400		13097700		13752600		37562300	23316600	965409	167676
6	97408900		13097700		13752600		38815100	24132700	994371	172707
7	102279000		13097700		13752600		40109900	24977300	1024200	177888
8	107393000		13097700		13752600		41448100	25851500	1054930	183224
9	112763000		13097700		13752600		42831100	26756300	1086580	188721
10	118401000		13097700		13752600		44260500	27692800	1119170	194383

Table G2. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	124321000		13097700		13752600		45737900	28662100	1152750	200214
12	130537000		13097700		13752600		47264800	29665200	1187330	206221
13	137064000		13097700		13752600		48842900	30703500	1222950	212407
14	143917000		13097700		13752600		50474000	31778100	1259640	218779
15	151113000		13097700		13752600		52159800	32890400	1297430	225343
16	158669000		13097700		13752600		53902200	34041500	1336350	232103
17	166602000		13097700		13752600		55703100	35233000	1376440	239066
18	174932000		13097700		13752600		57564500	36466100	1417740	246238
19	183679000		13097700		13752600		59488300	37742400	1460270	253625
20	192863000		13097700		13752600		61476800	39063400	1504080	261234

Table G2. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	3904850	98972	232323	14078800	1126310	-23774400	1047810	-24822200	0	-24822200
2	8714310	220871	518467	31520800	2521670	46096000	1047810	45048200	18019300	27028900
3	8975740	227498	534021	32571600	2605730	48968100	1047810	47920300	19168100	28752200
4	9245010	234322	550041	33657600	2692610	52002600	1047810	50954700	20381900	30572800
5	9522370	241352	566542	34779900	2782400	55208000	1047810	54160200	21664100	32496100
6	9808040	248593	583539	35939900	2875190	58593800	1047810	57546000	23018400	34527600
7	10102300	256051	601045	37138800	2971100	62169400	1047810	61121600	24448700	36673000
8	10405300	263732	619076	38377800	3070230	65945200	1047810	64897400	25959000	38938500
9	10717500	271644	637649	39658400	3172670	69931900	1047810	68884000	27553600	41330400
10	11039000	279793	656778	40982000	3278560	74140600	1047810	73092800	29237100	43855700

Table G2. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	11370200	288187	676481	42349900	3387990	78583300		78583300	31433300	47150000
12	11711300	296833	696776	43763700	3501100	83272400		83272400	33309000	49963500
13	12062600	305738	717679	45224900	3617990	88221200		88221200	35288500	52932700
14	12424500	314910	739209	46735200	3738820	93443300		93443300	37377300	56066000
15	12797300	324357	761386	48296100	3863690	98953300		98953300	39581300	59372000
16	13181200	334088	784227	49909500	3992760	104767000		104767000	41906600	62859900
17	13576600	344110	807754	51577000	4126160	110899000		110899000	44359700	66539500
18	13983900	354434	831987	53300400	4264040	117368000		117368000	46947200	70420700
19	14403400	365067	856946	55081800	4406540	124191000		124191000	49676300	74514400
20	14835500	376019	882655	56923000	4553840	131386000		131386000	52554500	78831700

Table G2. Economic analysis results of 30,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-23774400	29645300	-23774400	-19812000	-19812000
2	28076800	34042500	28076800	19497700	-314225
3	29800000	35177300	29800000	17245400	16931200
4	31620700	36350200	31620700	15249200	32180300
5	33543900	37562300	33543900	13480600	45660900
6	35575400	38815100	35575400	11914100	57575000
7	37720800	40109900	37720800	10527200	68102200
8	39986300	41448100	39986300	9299530	77401700
9	42378200	42831100	42378200	8213190	85614900
10	44903500	44260500	48177900	7252160	93395900

Table G2. Economic analysis results of 30,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	47150000	45737900		6345820	
12	49963500	47264800		5603730	
13	52932700	48842900		4947300	
14	56066000	50474000		4366790	
15	59372000	52159800		3853570	
16	62859900	53902200		3399960	
17	66539500	55703100		2999150	
18	70420700	57564500		2645080	
19	74514400	59488300		2332360	
20	78831700	61476800		2056250	

Table G3. Economic analysis results of 60,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.576923
DT (Duration of EPC Phase and Startup)	Period	0.961538
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	1.64E+07
RAWT (Total Raw Material Cost)	Cost/period	3.93E+07
PRODT (Total Product Sales)	Cost/period	1.45E+08
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.04E+06
UTILT (Total Utilities Cost)	Cost/period	1.64E+07
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G3. Economic analysis results of 60,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.25
OP (Total Operating Labor Cost)	Cost/period	832770
MT (Total Maintenance Cost)	Cost/period	211480

Table G3. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	5870940	18049100	16371000	17189600	17189600	859479	27122400	17193500	362896	92156
2	160277000		16371000		17189600		66250200	42061600	883486	224359
3	168291000		16371000		17189600		68464900	43533700	909990	231090
4	176705000		16371000		17189600		70753900	45057400	937290	238022
5	185540000		16371000		17189600		73119800	46634400	965409	245163
6	194817000		16371000		17189600		75565300	48266600	994371	252518
7	204558000		16371000		17189600		78092900	49956000	1024200	260093
8	214786000		16371000		17189600		80705400	51704400	1054930	267896
9	225526000		16371000		17189600		83405800	53514100	1086580	275933
10	236802000		16371000		17189600		86196900	55387100	1119170	284211

Table G3. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	248642000		16371000		17189600		89081900	57325600	1152750	292737
12	261074000		16371000		17189600		92063900	59332000	1187330	301520
13	274128000		16371000		17189600		95146300	61408600	1222950	310565
14	287834000		16371000		17189600		98332200	63557900	1259640	319882
15	302226000		16371000		17189600		101625000	65782500	1297430	329479
16	317337000		16371000		17189600		105029000	68084800	1336350	339363
17	333204000		16371000		17189600		108548000	70467800	1376440	349544
18	349864000		16371000		17189600		112185000	72934200	1417740	360030
19	367357000		16371000		17189600		115944000	75486900	1460270	370831
20	385725000		16371000		17189600		119830000	78128900	1504080	381956

Table G3. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	7146550	90724	227526	25113400	2009070	-39300500	1309680	-40610200	0	-40610200
2	17398600	220871	553922	61342800	4907430	94026500	1309680	92716800	37086700	55630100
3	17920600	227498	570540	63393400	5071470	99825700	1309680	98516000	39406400	59109600
4	18458200	234322	587656	65512900	5241030	105951000	1309680	104642000	41856600	62784900
5	19011900	241352	605286	67703600	5416280	112421000	1309680	111111000	44444300	66666500
6	19582300	248593	623444	69967800	5597430	119252000	1309680	117942000	47177000	70765500
7	20169800	256051	642148	72308200	5784660	126465000	1309680	125156000	50062300	75093400
8	20774800	263732	661412	74727200	5978180	134081000	1309680	132771000	53108400	79662700
9	21398100	271644	681255	77227600	6178210	142120000	1309680	140810000	56324000	84486000
10	22040000	279793	701692	79812000	6384960	150605000	1309680	149295000	59718100	89577100

Table G3. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	22701200	288187	722743	82483300	6598660	159560000		159560000	63824000	95736000
12	23382300	296833	744425	85244400	6819550	169010000		169010000	67604000	101406000
13	24083700	305738	766758	88098400	7047870	178981000		178981000	71592600	107389000
14	24806300	314910	789761	91048400	7283870	189502000		189502000	75800700	113701000
15	25550400	324357	813454	94097600	7527810	200600000		200600000	80240100	120360000
16	26317000	334088	837857	97249500	7779960	212308000		212308000	84923000	127385000
17	27106500	344110	862993	100507000	8040590	224656000		224656000	89862400	134794000
18	27919700	354434	888883	103875000	8309990	237679000		237679000	95071700	142607000
19	28757200	365067	915549	107356000	8588470	251413000		251413000	100565000	150848000
20	29620000	376019	943016	110954000	8876320	265895000		265895000	106358000	159537000

Table G3. Economic analysis results of 60,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-39300500	45171500	-39300500	-32750500	-32750500
2	56939800	66250200	56939800	39541500	6791060
3	60419300	68464900	60419300	34964900	41755900
4	64094600	70753900	64094600	30909800	72665800
5	67976200	73119800	67976200	27318100	99983900
6	72075200	75565300	72075200	24137800	124122000
7	76403100	78092900	76403100	21322700	145444000
8	80972300	80705400	80972300	18831600	164276000
9	85795700	83405800	85795700	16627800	180904000
10	90886800	86196900	94979500	14678700	196243000

Table G3. Economic analysis results of 60,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	95736000	89081900		12884900	
12	101406000	92063900		11373400	
13	107389000	95146300		10037000	
14	113701000	98332200		8855790	
15	120360000	101625000		7812040	
16	127385000	105029000		6889960	
17	134794000	108548000		6075580	
18	142607000	112185000		5356490	
19	150848000	115944000		4721670	
20	159537000	119830000		4161370	

Table G4. Economic analysis results of 90,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.596154
DT (Duration of EPC Phase and Startup)	Period	0.980769
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	1.93E+07
RAWT (Total Raw Material Cost)	Cost/period	5.89E+07
PRODT (Total Product Sales)	Cost/period	2.18E+08
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.11E+06
UTILT (Total Utilities Cost)	Cost/period	2.46E+07
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G4. Economic analysis results of 90,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.25
OP (Total Operating Labor Cost)	Cost/period	832770
MT (Total Maintenance Cost)	Cost/period	279416

Table G4. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	4403210	21238000	19263500	20226700	20226700	1011330	38473500	24617000	346400	116226
2	240415000		19263500		20226700		98454800	63090000	883486	296433
3	252436000		19263500		20226700		101749000	65298100	909990	305326
4	265058000		19263500		20226700		105154000	67583600	937290	314485
5	278311000		19263500		20226700		108674000	69949000	965409	323920
6	292226000		19263500		20226700		112312000	72397200	994371	333638
7	306838000		19263500		20226700		116072000	74931100	1024200	343647
8	322179000		19263500		20226700		119959000	77553700	1054930	353956
9	338288000		19263500		20226700		123976000	80268100	1086580	364575
10	355203000		19263500		20226700		128129000	83077400	1119170	375512

Table G4. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	372963000		19263500		20226700		132422000	85985200	1152750	386777
12	391611000		19263500		20226700		136859000	88994600	1187330	398381
13	411192000		19263500		20226700		141445000	92109400	1222950	410332
14	431751000		19263500		20226700		146186000	95333300	1259640	422642
15	453339000		19263500		20226700		151086000	98669900	1297430	435321
16	476006000		19263500		20226700		156151000	102123000	1336350	448381
17	499806000		19263500		20226700		161387000	105698000	1376440	461832
18	524796000		19263500		20226700		166800000	109397000	1417740	475687
19	551036000		19263500		20226700		172395000	113226000	1460270	489958
20	578588000		19263500		20226700		178178000	117189000	1504080	504657

Table G4. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	10226000	86600	231313	35623600	2849890	-55308300	1541080	-56849300	0	-56849300
2	26081100	220871	589959	91161900	7292950	141960000	1541080	140419000	56167800	84251600
3	26863600	227498	607658	94212200	7536970	150687000	1541080	149146000	59658300	89487500
4	27669500	234322	625888	97365000	7789200	159904000	1541080	158363000	63345000	95017500
5	28499600	241352	644664	100624000	8049910	169637000	1541080	168096000	67238300	100858000
6	29354600	248593	664004	103992000	8319390	179915000	1541080	178373000	71349400	107024000
7	30235200	256051	683924	107474000	8597930	190766000	1541080	189224000	75689800	113535000
8	31142300	263732	704442	111073000	8885840	202221000	1541080	200680000	80271800	120408000
9	32076500	271644	725575	114793000	9183440	214312000	1541080	212771000	85108400	127663000
10	33038800	279793	747343	118638000	9491050	227074000	1541080	225533000	90213100	135320000

Table G4. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	34030000	288187	769763	122613000	9809010	240541000		240541000	96216600	144325000
12	35050900	296833	792856	126721000	10137700	254753000		254753000	101901000	152852000
13	36102400	305738	816642	130968000	10477400	269747000		269747000	107899000	161848000
14	37185500	314910	841141	135357000	10828600	285566000		285566000	114226000	171339000
15	38301000	324357	866375	139894000	11191600	302253000		302253000	120901000	181352000
16	39450100	334088	892366	144585000	11566800	319854000		319854000	127942000	191913000
17	40633600	344110	919137	149433000	11954600	338419000		338419000	135367000	203051000
18	41852600	354434	946711	154444000	12355500	357997000		357997000	143199000	214798000
19	43108200	365067	975113	159625000	12770000	378642000		378642000	151457000	227185000
20	44401400	376019	1004370	164979000	13198400	400410000		400410000	160164000	240246000

Table G4. Economic analysis results of 90,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-55308300	59711500	-55308300	-46090200	-46090200
2	85792700	98454800	85792700	59578300	13488100
3	91028600	101749000	91028600	52678600	66166600
4	96558600	105154000	96558600	46565700	112732000
5	102399000	108674000	102399000	41151700	153884000
6	108565000	112312000	108565000	36358300	190242000
7	115076000	116072000	115076000	32115500	222358000
8	121949000	119959000	121949000	28361400	250719000
9	129204000	123976000	129204000	25040500	275760000
10	136861000	128129000	141677000	22103800	298641000

Table G4. Economic analysis results of 90,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	144325000	132422000		19424400	
12	152852000	136859000		17143300	
13	161848000	141445000		15127000	
14	171339000	146186000		13345000	
15	181352000	151086000		11770700	
16	191913000	156151000		10380200	
17	203051000	161387000		9152180	
18	214798000	166800000		8068030	
19	227185000	172395000		7111090	
20	240246000	178178000		6266590	

Table G5. Economic analysis results of 120,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.653846
DT (Duration of EPC Phase and Startup)	Period	1.03846
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	2.27E+07
RAWT (Total Raw Material Cost)	Cost/period	7.85E+07
PRODT (Total Product Sales)	Cost/period	2.91E+08
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.19E+06
UTILT (Total Utilities Cost)	Cost/period	3.28E+07
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G5. Economic analysis results of 120,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.25
OP (Total Operating Labor Cost)	Cost/period	832770
MT (Total Maintenance Cost)	Cost/period	357215

Table G5. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	0	25013300	22687800	23822200	23822200	1191110	43770100	28133900	296915	127361
2	308225000		22687800		23822200		130679000	84120300	883486	378969
3	336582000		22687800		23822200		135054000	87064500	909990	390338
4	353411000		22687800		23822200		139576000	90111800	937290	402048
5	371081000		22687800		23822200		144249000	93265700	965409	414110
6	389635000		22687800		23822200		149080000	96530000	994371	426533
7	409117000		22687800		23822200		154074000	99908500	1024200	439329
8	429573000		22687800		23822200		159236000	103405000	1054930	452509
9	451052000		22687800		23822200		164571000	107025000	1086580	466084
10	473604000		22687800		23822200		170086000	110770000	1119170	480066

Table G5. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	497285000		22687800		23822200		175787000	114647000	1152750	494468
12	522149000		22687800		23822200		181680000	118660000	1187330	509302
13	548256000		22687800		23822200		187771000	122813000	1222950	524582
14	575669000		22687800		23822200		194067000	127112000	1259640	540319
15	604452000		22687800		23822200		200576000	131560000	1297430	556529
16	634675000		22687800		23822200		207304000	136165000	1336350	573224
17	666409000		22687800		23822200		214258000	140931000	1376440	590421
18	699729000		22687800		23822200		221447000	145863000	1417740	608134
19	734716000		22687800		23822200		228878000	150969000	1460270	626378
20	771452000		22687800		23822200		236559000	156253000	1504080	645169

Table G5. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	11683300	74229	212138	40527800	3242230	-68783400	1815030	-70598400	0	-70598400
2	34764300	220871	631227	120999000	9679940	177546000	1815030	175731000	70292400	105439000
3	35807300	227498	650164	125050000	10004000	201528000	1815030	199713000	79885200	119828000
4	36881500	234322	669669	129237000	10338900	213835000	1815030	212020000	84808100	127212000
5	37987900	241352	689759	133564000	10685100	226832000	1815030	225017000	90006800	135010000
6	39127600	248593	710452	138037000	11043000	240555000	1815030	238740000	95496000	143244000
7	40301400	256051	731765	142661000	11412900	255043000	1815030	253228000	101291000	151937000
8	41510400	263732	753718	147441000	11795300	270337000	1815030	268522000	107409000	161113000
9	42755700	271644	776330	152381000	12190500	286480000	1815030	284665000	113866000	170799000
10	44038400	279793	799620	157487000	12599000	303518000	1815030	301703000	120681000	181022000

Table G5. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	45359600	288187	823608	162766000	13021300	321497000		321497000	128599000	192898000
12	46720300	296833	848317	168222000	13457800	340469000		340469000	136188000	204281000
13	48122000	305738	873766	173862000	13909000	360485000		360485000	144194000	216291000
14	49565600	314910	899979	179692000	14375400	381602000		381602000	152641000	228961000
15	51052600	324357	926979	185718000	14857500	403877000		403877000	161551000	242326000
16	52584200	334088	954788	191948000	15355800	427372000		427372000	170949000	256423000
17	54161700	344110	983432	198387000	15871000	452151000		452151000	180860000	271291000
18	55786500	354434	1012930	205043000	16403500	478283000		478283000	191313000	286970000
19	57460100	365067	1043320	211924000	16953900	505838000		505838000	202335000	303503000
20	59183900	376019	1074620	219036000	17522900	534892000		534892000	213957000	320935000

Table G5. Economic analysis results of 120,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-68783400	68783400	-68783400	-57319500	-57319500
2	107254000	130679000	107254000	74481600	17162100
3	121643000	135054000	121643000	70395100	87557300
4	129027000	139576000	129027000	62223800	149781000
5	136825000	144249000	136825000	54987000	204768000
6	145059000	149080000	145059000	48580000	253348000
7	153752000	154074000	153752000	42909300	296257000
8	162928000	159236000	162928000	37891900	334149000
9	172614000	164571000	172614000	33453800	367603000
10	182837000	170086000	188509000	29529200	398048000

Table G5. Economic analysis results of 120,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	192898000	175787000		25961800	
12	204281000	181680000		22911500	
13	216291000	187771000		20215400	
14	228961000	194067000		17833000	
15	242326000	200576000		15728300	
16	256423000	207304000		13869400	
17	271291000	214258000		12227900	
18	286970000	221447000		10778900	
19	303503000	228878000		9499900	
20	320935000	236559000		8371290	

G.2 Acetaldehyde production at 300°C

Table G6. Economic analysis results of 12,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.461538
DT (Duration of EPC Phase and Startup)	Period	0.846154
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	1.05E+07
RAWT (Total Raw Material Cost)	Cost/period	1.40E+07
PRODT (Total Product Sales)	Cost/period	2.21E+07
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.11E+06
UTILT (Total Utilities Cost)	Cost/period	1.62E+06
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5

Table G6. Economic analysis results of 12,000 tons/year (Cont'd)

ITEM	UNITS	
ESRAW (Raw Material Escalation)	Percent/period	3.5
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.192308
OP (Total Operating Labor Cost)	Cost/period	1.01E+06
MT (Total Maintenance Cost)	Cost/period	103220

Table G6. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	3571490	11529100	10457300	10980100	10980100	549006	10529500	7786210	559102	57247
2	24375400		10457300		10980100		20219600	14966200	1069480	109506
3	25594200		10457300		10980100		20907000	15490000	1101570	112791
4	26873900		10457300		10980100		21617800	16032200	1134610	116175
5	28217600		10457300		10980100		22353000	16593300	1168650	119660
6	29628500		10457300		10980100		23113100	17174100	1203710	123250
7	31109900		10457300		10980100		23899300	17775200	1239820	126947
8	32665400		10457300		10980100		24712200	18397300	1277020	130756
9	34298700		10457300		10980100		25553000	19041200	1315330	134678
10	36013600		10457300		10980100		26422400	19707600	1354790	138719

Table G6. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	37814300		10457300		10980100		27321500	20397400	1395430	142880
12	39705000		10457300		10980100		28251200	21111300	1437300	147167
13	41690200		10457300		10980100		29212800	21850200	1480410	151582
14	43774700		10457300		10980100		30207200	22615000	1524830	156129
15	45963500		10457300		10980100		31235500	23406500	1570570	160813
16	48261700		10457300		10980100		32299000	24225700	1617690	165637
17	50674700		10457300		10980100		33398700	25073600	1666220	170606
18	53208500		10457300		10980100		34536100	25951200	1716210	175725
19	55868900		10457300		10980100		35712300	26859500	1767690	180996
20	58662300		10457300		10980100		36928700	27799600	1820720	186426

Table G6. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	899064	139776	308175	9749570	779966	-18487200	836581	-19323800	0	-19323800
2	1719780	267371	589494	18721800	1497750	4155840	836581	3319260	1327700	1991550
3	1771370	275392	607179	19358300	1548670	4687200	836581	3850620	1540250	2310370
4	1824520	283654	625394	20016500	1601320	5256060	836581	4419470	1767790	2651680
5	1879250	292163	644156	20697200	1655770	5864640	836581	5028060	2011220	3016840
6	1935630	300928	663481	21401100	1712080	6515330	836581	5678750	2271500	3407250
7	1993700	309956	683385	22129000	1770320	7210620	836581	6374040	2549610	3824420
8	2053510	319255	703887	22881700	1830540	7953150	836581	7116570	2846630	4269940
9	2115110	328832	725004	23660100	1892810	8745710	836581	7909120	3163650	4745470
10	2178570	338697	746754	24465200	1957210	9591230	836581	8754650	3501860	5252790

Table G6. Economic analysis results of 12,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	2243920	348858	769156	25297600	2023810	10492800		10492800	4197130	6295690
12	2311240	359324	792231	26158600	2092680	11453700		11453700	4581500	6872240
13	2380580	370104	815998	27048900	2163910	12477400		12477400	4990980	7486470
14	2452000	381207	840478	27969600	2237570	13567600		13567600	5427030	8140550
15	2525560	392643	865692	28921800	2313740	14728000		14728000	5891200	8836790
16	2601320	404422	891663	29906400	2392520	15962700		15962700	6385080	9577620
17	2679360	416555	918413	30924800	2473980	17276000		17276000	6910400	10365600
18	2759740	429051	945965	31977900	2558230	18672400		18672400	7468950	11203400
19	2842540	441923	974344	33067000	2645360	20156600		20156600	8062630	12093900
20	2927810	455181	1003570	34193300	2735460	21733600		21733600	8693450	13040200

Table G6. Economic analysis results of 12,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-18487200	22058700	-18487200	-15406000	-15406000
2	2828130	20219600	2828130	1963980	-13442000
3	3146950	20907000	3146950	1821150	-11620800
4	3488270	21617800	3488270	1682230	-9938610
5	3853420	22353000	3853420	1548600	-8390010
6	4243830	23113100	4243830	1421250	-6968760
7	4661000	23899300	4661000	1300800	-5667960
8	5106520	24712200	5106520	1187610	-4480350
9	5582060	25553000	5582060	1081840	-3398510
10	6089370	26422400	8703680	983467	-1992820

Table G6. Economic analysis results of 12,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	6295690	27321500		847324	
12	6872240	28251200		770768	
13	7486470	29212800		699714	
14	8140550	30207200		634040	
15	8836790	31235500		573556	
16	9577620	32299000		518033	
17	10365600	33398700		467211	
18	11203400	34536100		420812	
19	12093900	35712300		378551	
20	13040200	36928700		340140	

Table G7. Economic analysis results of 30,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.480769
DT (Duration of EPC Phase and Startup)	Period	0.865385
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	1.43E+07
RAWT (Total Raw Material Cost)	Cost/period	3.49E+07
PRODT (Total Product Sales)	Cost/period	5.53E+07
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.20E+06
UTILT (Total Utilities Cost)	Cost/period	4.06E+06
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G7. Economic analysis results of 30,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.192308
OP (Total Operating Labor Cost)	Cost/period	1.01E+06
MT (Total Maintenance Cost)	Cost/period	196139

Table G7. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	7812630	15736100	14273100	14986700	14986700	749336	23803800	18770300	539134	104897
2	60938500		14273100		14986700		47414900	37415500	1069480	208084
3	63985400		14273100		14986700		49039400	38725000	1101570	214327
4	67184700		14273100		14986700		50719700	40080400	1134610	220756
5	70543900		14273100		14986700		52457700	41483200	1168650	227379
6	74071100		14273100		14986700		54255500	42935100	1203710	234201
7	77774700		14273100		14986700		56115000	44437900	1239820	241227
8	81663400		14273100		14986700		58038400	45993200	1277020	248463
9	85746600		14273100		14986700		60027900	47602900	1315330	255917
10	90033900		14273100		14986700		62085800	49269000	1354790	263595

Table G7. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	94535600		14273100		14986700		64214400	50993500	1395430	271503
12	99262400		14273100		14986700		66416200	52778200	1437300	279648
13	104226000		14273100		14986700		68693700	54625500	1480410	288037
14	109437000		14273100		14986700		71049500	56537400	1524830	296678
15	114909000		14273100		14986700		73486300	58516200	1570570	305579
16	120654000		14273100		14986700		76006900	60564200	1617690	314746
17	126687000		14273100		14986700		78614100	62684000	1666220	324188
18	133021000		14273100		14986700		81311000	64877900	1716210	333914
19	139672000		14273100		14986700		84100700	67148600	1767690	343931
20	146656000		14273100		14986700		86986300	69498800	1820720	354249

Table G7. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	2169420	134784	322016	22040600	1763240	-31727200	1141850	-32869100	0	-32869100
2	4303500	267371	638783	43902700	3512220	13523600	1141850	12381700	4952690	7429040
3	4432600	275392	657947	45406900	3632550	14946000	1141850	13804200	5521670	8282500
4	4565580	283654	677685	46962700	3757010	16465000	1141850	15323100	6129260	9193890
5	4702550	292163	698016	48572000	3885760	18086200	1141850	16944400	6777740	10166600
6	4843620	300928	718956	50236500	4018920	19815700	1141850	18673800	7469520	11204300
7	4988930	309956	740525	51958300	4156670	21659700	1141850	20517900	8207140	12310700
8	5138600	319255	762741	53739300	4299140	23625000	1141850	22483200	8993270	13489900
9	5292760	328832	785623	55581400	4446510	25718700	1141850	24576800	9830730	14746100
10	5451540	338697	809192	57486900	4598950	27948100	1141850	26806300	10722500	16083800

Table G7. Economic analysis results of 30,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	5615090	348858	833467	59457800	4756620	30321200		30321200	12128500	18192700
12	5783540	359324	858471	61496500	4919720	32846200		32846200	13138500	19707700
13	5957040	370104	884226	63605300	5088420	35531800		35531800	14212700	21319100
14	6135760	381207	910752	65786600	5262930	38387300		38387300	15354900	23032400
15	6319830	392643	938075	68042900	5443430	41422300		41422300	16568900	24853400
16	6509420	404422	966217	70376700	5630140	44647200		44647200	17858900	26788300
17	6704710	416555	995204	72790900	5823270	48072600		48072600	19229100	28843600
18	6905850	429051	1025060	75288000	6023040	51710100		51710100	20684000	31026000
19	7113020	441923	1055810	77871000	6229680	55571400		55571400	22228600	33342900
20	7326410	455181	1087490	80542900	6443430	59669400		59669400	23867800	35801700

Table G7. Economic analysis results of 30,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-31727200	39539900	-31727200	-26439400	-26439400
2	8570890	47414900	8570890	5952000	-20487400
3	9424350	49039400	9424350	5453900	-15033500
4	10335700	50719700	10335700	4984440	-10049000
5	11308500	52457700	11308500	4544620	-5504400
6	12346100	54255500	12346100	4134690	-1369700
7	13452600	56115000	13452600	3754360	2384660
8	14631700	58038400	14631700	3402880	5787540
9	15887900	60027900	15887900	3079190	8866720
10	17225600	62085800	20793900	2782030	12225100

Table G7. Economic analysis results of 30,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	18192700	64214400		2448520	
12	19707700	66416200		2210350	
13	21319100	68693700		1992560	
14	23032400	71049500		1793910	
15	24853400	73486300		1613120	
16	26788300	76006900		1448920	
17	28843600	78614100		1300070	
18	31026000	81311000		1165370	
19	33342900	84100700		1043660	
20	35801700	86986300		933852	

Table G8. Economic analysis results of 60,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.5
DT (Duration of EPC Phase and Startup)	Period	0.884615
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	2.44E+07
RAWT (Total Raw Material Cost)	Cost/period	6.99E+07
PRODT (Total Product Sales)	Cost/period	1.11E+08
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.46E+06
UTILT (Total Utilities Cost)	Cost/period	8.09E+06
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G8. Economic analysis results of 60,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.211538
OP (Total Operating Labor Cost)	Cost/period	1.01E+06
MT (Total Maintenance Cost)	Cost/period	453641

Table G8. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	13393100	26924800	24421600	25642700	25642700	1282130	44900100	36150200	519166	233625
2	121877000		24421600		25642700		92884600	74831000	1069480	481267
3	127971000		24421600		25642700		96075300	77450100	1101570	495705
4	134369000		24421600		25642700		99375800	80160800	1134610	510576
5	141088000		24421600		25642700		102790000	82966400	1168650	525894
6	148142000		24421600		25642700		106322000	85870300	1203710	541670
7	155549000		24421600		25642700		109975000	88875700	1239820	557921
8	163327000		24421600		25642700		113754000	91986400	1277020	574658
9	171493000		24421600		25642700		117663000	95205900	1315330	591898
10	180068000		24421600		25642700		121708000	98538100	1354790	609655

Table G8. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	189071000		24421600		25642700		125891000	101987000	1395430	627945
12	198525000		24421600		25642700		130218000	105556000	1437300	646783
13	208451000		24421600		25642700		134695000	109251000	1480410	666186
14	218874000		24421600		25642700		139326000	113075000	1524830	686172
15	229817000		24421600		25642700		144116000	117032000	1570570	706757
16	241308000		24421600		25642700		149071000	121128000	1617690	727960
17	253373000		24421600		25642700		154198000	125368000	1666220	749799
18	266042000		24421600		25642700		159501000	129756000	1716210	772293
19	279344000		24421600		25642700		164986000	134297000	1767690	795461
20	293311000		24421600		25642700		170661000	138998000	1820720	819325

Table G8. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	4164960	129792	376396	41574200	3325930	-58431900	1953730	-60385600	0	-60385600
2	8579820	267371	775375	86004300	6880340	28992300	1953730	27038600	10815400	16223200
3	8837220	275392	798636	88958600	7116690	31895600	1953730	29941800	11976700	17965100
4	9102330	283654	822595	92014600	7361170	34993600	1953730	33039900	13216000	19823900
5	9375400	292163	847273	95175800	7614070	38297900	1953730	36344200	14537700	21806500
6	9656660	300928	872691	98445900	7875670	41820600	1953730	39866900	15946800	23920100
7	9946360	309956	898872	101829000	8146290	45574400	1953730	43620700	17448300	26172400
8	10244800	319255	925838	105328000	8426230	49572700	1953730	47618900	19047600	28571400
9	10552100	328832	953613	108948000	8715810	53829700	1953730	51875900	20750400	31125600
10	10868700	338697	982222	112692000	9015370	58360300	1953730	56406600	22562600	33843900

Table G8. Economic analysis results of 60,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	11194700	348858	1011690	116566000	9325250	63180400		63180400	25272100	37908200
12	11530600	359324	1042040	120572000	9645800	68306500		68306500	27322600	40983900
13	11876500	370104	1073300	124717000	9977400	73756200		73756200	29502500	44253700
14	12232800	381207	1105500	129005000	10320400	79547900		79547900	31819200	47728700
15	12599800	392643	1138660	133441000	10675300	85701200		85701200	34280500	51420700
16	12977700	404422	1172820	138029000	11042300	92236600		92236600	36894600	55342000
17	13367100	416555	1208010	142776000	11422100	99175800		99175800	39670300	59505500
18	13768100	429051	1244250	147686000	11814900	106542000		106542000	42616600	63924900
19	14181100	441923	1281580	152765000	12221200	114358000		114358000	45743200	68614800
20	14606600	455181	1320020	158020000	12641600	122650000		122650000	49060100	73590200

Table G8. Economic analysis results of 60,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-58431900	71824900	-58431900	-48693200	-48693200
2	18176900	92884600	18176900	12622800	-36070400
3	19918800	96075300	19918800	11527100	-24543300
4	21777700	99375800	21777700	10502300	-14040900
5	23760300	102790000	23760300	9548720	-4492210
6	25873900	106322000	25873900	8665110	4172900
7	28126100	109975000	28126100	7849490	12022400
8	30525100	113754000	30525100	7099160	19121500
9	33079300	117663000	33079300	6410990	25532500
10	35797700	121708000	41903100	5781520	32300100

Table G8. Economic analysis results of 60,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	37908200	125891000		5101990	
12	40983900	130218000		4596620	
13	44253700	134695000		4136120	
14	47728700	139326000		3717430	
15	51420700	144116000		3337490	
16	55342000	149071000		2993330	
17	59505500	154198000		2682100	
18	63924900	159501000		2401090	
19	68614800	164986000		2147700	
20	73590200	170661000		1919530	

Table G9. Economic analysis results of 90,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.519231
DT (Duration of EPC Phase and Startup)	Period	0.903846
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	3.28E+07
RAWT (Total Raw Material Cost)	Cost/period	1.05E+08
PRODT (Total Product Sales)	Cost/period	1.66E+08
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.67E+06
UTILT (Total Utilities Cost)	Cost/period	1.19E+07
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G9. Economic analysis results of 90,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.211538
OP (Total Operating Labor Cost)	Cost/period	1.01E+06
MT (Total Maintenance Cost)	Cost/period	664025

Table G9. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	16741300	36146300	32785800	34425000	34425000	1721250	64155800	52139800	499198	328820
2	182815000		32785800		34425000		138033000	112246000	1069480	704464
3	191956000		32785800		34425000		142780000	116175000	1101570	725597
4	201554000		32785800		34425000		147691000	120241000	1134610	747365
5	211632000		32785800		34425000		152771000	124450000	1168650	769786
6	222213000		32785800		34425000		158026000	128805000	1203710	792880
7	233324000		32785800		34425000		163462000	133314000	1239820	816666
8	244990000		32785800		34425000		169086000	137980000	1277020	841166
9	257240000		32785800		34425000		174904000	142809000	1315330	866401
10	270102000		32785800		34425000		180922000	147807000	1354790	892393

Table G9. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	283607000		32785800		34425000		187148000	152980000	1395430	919165
12	297787000		32785800		34425000		193588000	158335000	1437300	946740
13	312676000		32785800		34425000		200251000	163876000	1480410	975142
14	328310000		32785800		34425000		207144000	169612000	1524830	1004400
15	344726000		32785800		34425000		214274000	175549000	1570570	1034530
16	361962000		32785800		34425000		221650000	181693000	1617690	1065560
17	380060000		32785800		34425000		229281000	188052000	1666220	1097530
18	399063000		32785800		34425000		237175000	194634000	1716210	1130460
19	419016000		32785800		34425000		245341000	201446000	1767690	1164370
20	439967000		32785800		34425000		253789000	208497000	1820720	1199300

Table G9. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	5896940	124800	414009	59403500	4752280	-83560800	2622860	-86183600	0	-86183600
2	12633600	267371	886973	127808000	10224700	44782400	2622860	42159500	16863800	25295700
3	13012600	275392	913582	132204000	10576300	49176000	2622860	46553100	18621300	27931900
4	13403000	283654	940990	136751000	10940100	53863100	2622860	51240200	20496100	30744100
5	13805100	292163	969219	141455000	11316400	58860700	2622860	56237900	22495100	33742700
6	14219200	300928	998296	146320000	11705600	64187200	2622860	61564300	24625700	36938600
7	14645800	309956	1028240	151354000	12108300	69861500	2622860	67238600	26895500	40343200
8	15085200	319255	1059090	156561000	12524900	75903900	2622860	73281100	29312400	43968600
9	15537700	328832	1090870	161948000	12955800	82335800	2622860	79712900	31885200	47827700
10	16003900	338697	1123590	167520000	13401600	89179400	2622860	86556600	34622600	51934000

Table G9. Economic analysis results of 90,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	16484000	348858	1157300	173285000	13862800	96458700		96458700	38583500	57875200
12	16978500	359324	1192020	179249000	14339900	104199000		104199000	41679400	62519100
13	17487900	370104	1227780	185418000	14833400	112425000		112425000	44970100	67455100
14	18012500	381207	1264610	191800000	15344000	121167000		121167000	48466600	72699900
15	18552900	392643	1302550	198402000	15872100	130452000		130452000	52180700	78271100
16	19109500	404422	1341630	205231000	16418500	140312000		140312000	56124800	84187200
17	19682700	416555	1381880	212297000	16983800	150779000		150779000	60311800	90467600
18	20273200	429051	1423330	219606000	17568500	161889000		161889000	64755400	97133100
19	20881400	441923	1466030	227167000	18173400	173675000		173675000	69470200	104205000
20	21507900	455181	1510010	234990000	18799200	186178000		186178000	74471300	111707000

Table G9. Economic analysis results of 90,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-83560800	100302000	-83560800	-69634000	-69634000
2	27918600	138033000	27918600	19387900	-50246100
3	30554700	142780000	30554700	17682100	-32563900
4	33367000	147691000	33367000	16091300	-16472600
5	36365600	152771000	36365600	14614500	-1858090
6	39561400	158026000	39561400	13249000	11391000
7	42966000	163462000	42966000	11991000	23382000
8	46591500	169086000	46591500	10835700	34217700
9	50450600	174904000	50450600	9777660	43995300
10	54556800	180922000	62753300	8811230	54130300

Table G9. Economic analysis results of 90,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	57875200	187148000		7789310	
12	62519100	193588000		7011930	
13	67455100	200251000		6304620	
14	72699900	207144000		5662350	
15	78271100	214274000		5080220	
16	84187200	221650000		4553510	
17	90467600	229281000		4077670	
18	97133100	237175000		3648420	
19	104205000	245341000		3261710	
20	111707000	253789000		2913770	

Table G10. Economic analysis results of 120,000 tons/year

ITEM	UNITS	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.519231
DT (Duration of EPC Phase and Startup)	Period	0.903846
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	4.13E+07
RAWT (Total Raw Material Cost)	Cost/period	1.40E+08
PRODT (Total Product Sales)	Cost/period	2.21E+08
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.90E+06
UTILT (Total Utilities Cost)	Cost/period	1.57E+07
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5

Table G10. Economic analysis results of 120,000 tons/year (Cont'd)

ITEM	UNITS	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.211538
OP (Total Operating Labor Cost)	Cost/period	1.01E+06
MT (Total Maintenance Cost)	Cost/period	895228

Table G10. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
0	0	0	0	0	0	0	0	0	0	0
1	22321800	45556600	41321200	43387200	43387200	2169360	85153600	69519700	499198	443310
2	243754000		41321200		43387200		183214000	149662000	1069480	949747
3	255942000		41321200		43387200		189519000	154900000	1101570	978240
4	268739000		41321200		43387200		196041000	160322000	1134610	1007590
5	282176000		41321200		43387200		202788000	165933000	1168650	1037810
6	296284000		41321200		43387200		209767000	171741000	1203710	1068950
7	311099000		41321200		43387200		216988000	177751000	1239820	1101020
8	326654000		41321200		43387200		224457000	183973000	1277020	1134050
9	342986000		41321200		43387200		232184000	190412000	1315330	1168070
10	360135000		41321200		43387200		240178000	197076000	1354790	1203110

Table G10. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Sales (Cost/Period)	Expenses (Cost/Period)								
	SP (Products Sales)	CAP (Capital Costs)	Unescalated Cumulative Capital Cost	Capital Cost	Cumulative Capital Cost	Working Capital	OP (Operating Costs)	Raw Materials	Operating Labor Cost	Maintenance Cost
11	378142000		41321200		43387200		248448000	203974000	1395430	1239200
12	397049000		41321200		43387200		257003000	211113000	1437300	1276380
13	416902000		41321200		43387200		265853000	218502000	1480410	1314670
14	437747000		41321200		43387200		275008000	226149000	1524830	1354110
15	459634000		41321200		43387200		284480000	234065000	1570570	1394740
16	482616000		41321200		43387200		294278000	242257000	1617690	1436580
17	506747000		41321200		43387200		304414000	250736000	1666220	1479680
18	532084000		41321200		43387200		314901000	259512000	1716210	1524070
19	558688000		41321200		43387200		325749000	268595000	1767690	1569790
20	586623000		41321200		43387200		336972000	277995000	1820720	1616880

Table G10. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
0	0	0	0	0	0	0	0	0	0	0
1	7787730	124800	471254	78846000	6307680	-108388000	3305690	-111694000	0	-111694000
2	16684400	267371	1009610	169643000	13571400	60539900	3305690	57234200	22893700	34340500
3	17185000	275392	1039900	175480000	14038400	66423000	3305690	63117300	25246900	37870400
4	17700500	283654	1071100	181519000	14521500	72698000	3305690	69392300	27756900	41635400
5	18231500	292163	1103230	187766000	15021300	79388000	3305690	76082300	30432900	45649400
6	18778500	300928	1136330	194229000	15538300	86517100	3305690	83211400	33284600	49926900
7	19341800	309956	1170420	200914000	16073200	94110900	3305690	90805200	36322100	54483100
8	19922100	319255	1205530	207831000	16626500	102196000	3305690	98890700	39556300	59334400
9	20519700	328832	1241700	214985000	17198800	110802000	3305690	107496000	42998500	64497700
10	21135300	338697	1278950	222387000	17791000	119957000	3305690	116652000	46660700	69991000

Table G10. Economic analysis results of 120,000 tons/year (Cont'd)

Year	Expenses (Cost/Period)					R (Revenue)	DEP (Depreciation Expense)	E (Earnings Before Taxes)	TAX (Taxes)	NE (Net Earnings)
	Utilities	Operating Charges	Plant Overhead	Subtotal Operating Costs	G and A Costs					
11	21769400	348858	1317320	230044000	18403500	129695000		129695000	51877900	77816800
12	22422500	359324	1356840	237965000	19037200	140047000		140047000	56018700	84028100
13	23095100	370104	1397540	246160000	19692800	151049000		151049000	60419700	90629600
14	23788000	381207	1439470	254637000	20371000	162739000		162739000	65095500	97643300
15	24501600	392643	1482650	263407000	21072600	175155000		175155000	70061900	105093000
16	25236700	404422	1527130	272480000	21798400	188338000		188338000	75335300	113003000
17	25993800	416555	1572950	281865000	22549200	202332000		202332000	80933000	121399000
18	26773600	429051	1620140	291575000	23326000	217183000		217183000	86873300	130310000
19	27576800	441923	1668740	301620000	24129600	232939000		232939000	93175700	139763000
20	28404100	455181	1718800	312011000	24960900	249651000		249651000	99860300	149790000

Table G10. Economic analysis results of 120,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
0	0	0	0	0	0
1	-108388000	130710000	-108388000	-90323700	-90323700
2	37646200	183214000	37646200	26143200	-64180500
3	41176100	189519000	41176100	23828700	-40351800
4	44941100	196041000	44941100	21673000	-18678800
5	48955100	202788000	48955100	19673900	995163
6	53232500	209767000	53232500	17827500	18822600
7	57788800	216988000	57788800	16127800	34950400
8	62640100	224457000	62640100	14568100	49518500
9	67803400	232184000	67803400	13140800	62659300
10	73296700	240178000	83627000	11837800	76165500

Table G10. Economic analysis results of 120,000 tons/year (Cont'd)

Year	TED (Total Earnings)	TEX (Total Expenses (Excludes Taxes and Depreciation))	CF (Cash Flow for Project)	PV (Present Value of Cash Flows)	NPV (Net Present Value)
11	77816800	248448000		10473200	
12	84028100	257003000		9424310	
13	90629600	265853000		8470590	
14	97643300	275008000		7605100	
15	105093000	284480000		6821100	
16	113003000	294278000		6112090	
17	121399000	304414000		5471870	
18	130310000	314901000		4894580	
19	139763000	325749000		4374720	
20	149790000	336972000		3907140	

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