Economic evaluation of Ethyl lactate production via reactive distillation at different concentrations of lactic acid

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การประเมินทางเศรษฐศาสตร์ของกระบวนการผลิตเอทิลแลคเตทผ่านการกลั่นแบบมีปฏิกิริยาร่วมด้วยที่ความเข้มข้นแตกต่างกันของกรดแลคติก

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เอทิลแลคเตทเป็นตัวทำละลายชีวภาพที่ผลิตจากพืชผลทางการเกษตร ทำให้เป็นมิตรต่อสิ่งแวดล้อมมากกว่าตัวทำละลายปิโตรเคมี ผลิตภัณฑ์ได้มาจากการเอสเทอริฟิเคชันของกรดแลกติกด้วยเอทานอลโดยใช้ตัวเร่งปฏิกิริยากรดแอมเบอร์ลิสท์-15 ในหอกลั่นแบบมีปฏิกิริยาร่วมด้วย

ในการผลิตเอทิลแลคเตทในเชิงอุตสาหกรรม งานนี้ออกแบบกระบวนการผลิตที่ความเข้มข้นของกรดแลคติกสองระดับ (ร้อยละ 50 และ 85 โดยน้ำหนัก) และอุณหภูมิป้อนเอทานอลสองระดับ (25 และ 85 °C) กรดแลคติกที่มีความเข้มข้นสูงสามารถทำให้เกิดผลเสีย เช่น ปริมาณโอลิโกเมอร์เพิ่มขึ้นและผลิตภัณฑ์ที่ต้องการลดลง ทำให้การจำลองกระบวนการผลิตที่ครอบคลุมจำเป็นในการประเมินการใช้พลังงาน เศรษฐศาสตร์ และการปล่อยก๊าซคาร์บอนไดออกไซด์

ผลการจำลองแสดงให้เห็นว่ากระบวนการผลิตเอทิลแลคเตทที่ร้อยละ 85 โดยน้ำหนักของกรดแลคติกและ 25 °C ของอุณหภูมิป้อนเอทานอลเป็นกรณีที่ดีที่สุด โดยมูลค่าปัจจุบันสุทธิ 176 ล้านเหรียญสหรัฐฯ อัตราผลตอบแทนภายในที่ 74.6% ระยะเวลาคืนทุน 3.41 ปี ปริมาณการใช้พลังงานต่อหนึ่งหน่วยการผลิต 2.60 kWh/kg L_1E และการปล่อยก๊าซคาร์บอนไดออกไซด์ต่อหนึ่งหน่วยการผลิต 1.91 kg $CO_{2\text{-eq}}$/kg L_1E กระบวนการนี้ประหยัดพลังงานมากกว่าและมีการปล่อยก๊าซคาร์บอนไดออกไซด์ต่ำกว่าเมื่อเทียบกับการผลิตเอทิลแลคเตทที่ร้อยละ 50 โดยน้ำหนักของกรดแลคติก

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Ethyl lactate is a green solvent made from agricultural crops, making it more environmentally friendly than petrochemical solvents. The product is obtained via esterification of lactic acid with ethanol over Amberlyst-15 acid catalyst in a reactive distillation column.

In commercial-scale production of ethyl lactate, this work designs production processes at two concentrations of lactic acid (50 and 85 wt.%) and two ethanol feed temperatures (25 and 85 °C). Highly concentrated lactic acid can result in adverse effects, such as increased oligomers and reduced desired products, making a comprehensive simulation of the production process necessary to evaluate energy consumption, economics, and CO_2 emissions.

The simulation results show that the ethyl lactate production process at 85 wt.% of lactic acid and 25 °C of ethanol feed temperature is the best scenario, with a net present value of 176 million USD, internal rate of return of 74.6%, payout period of 3.41 years, specific energy consumption of 2.60 kWh/kg L_1E, and CO_2 emissions of 1.91 kg $CO_{2\text{-eq}}$/kg L_1E. This process is more energy-efficient and has lower CO_2 emissions compared to producing ethyl lactate at 50 wt.% of lactic acid.

Field of Study: Chemical Engineering Student's Signature .....

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Nattapat Klin-u-bol

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CHAPTER I

INTRODUCTION

1.1 Background

Solvents are one of the most chemicals used in the chemical industry. The solvents can be classified into two types, biosolvents and petrochemical solvents, according to the raw materials used to produce them. The biosolvents or green solvents, which are produced from agricultural crops, are more environmentally friendly than the petrochemical solvents. Thus, the green solvents are a new alternative without severe effects on the environment.[1]

Ethyl lactate is a green solvent derived from esterifying ethanol and lactic acid. It's easily biodegradable and has various applications including as a cleaning agent, food additive, and flavor chemical. Its main use is as a solvent in the electronic industry and it can replace hazardous solvents like perchloroethylene, halogenated solvents, methylene chloride, chloroform, and ethyl glycol ethers on a 1:1 basis.[2]

The global market size of ethyl lactate is currently being analyzed and forecasted for the period between 2021 and 2026 by the chemical research industry. The global market revenue for ethyl lactate in 2022 was 86 million USD. The market is expected to reach a size of 107.5 million USD by 2026, with an average annual growth rate of 3.2% during the forecast period 2023-2028.[3] This represents a promising opportunity for investment in the market as a means to reduce reliance on solvents derived from crude oil.

There are many types of esterification processes, such as pervaporation membrane, reactive distillation, chromatographic reactors, etc. The most popular production process is the reactive distillation process. The reactive distillation consists of both separation and reaction in one unit operation. The reactive distillation column is divided into 3 sections: a nonreactive stripping section, a reactive section, and a nonreactive enriching section. The main chemical reaction for

ethyl lactate production from esterification of ethanol and lactic acid occurs over Amberlyst-15 cation exchange resin catalyst packed in the reactive section.[4]

In this project, two different concentrations of lactic acid solution, which is the main raw material for ethyl lactate production, are used to simulate by a process simulation program, namely Aspen plus and Aspen economic analysis. Different concentrations of the lactic acid solution mean different components. From the bifunctional nature of lactic acid. If a highly concentrated form of lactic acid is utilized, it may yield adverse effects in addition to its costly nature. Specifically, there may be an increase in the number of oligomers, which could lead to a reduction in the overall quantity of the desired product or even negatively impact the production process itself. To mitigate such potential issues, it is imperative that we undertake a comprehensive simulation of the production process to evaluate and optimize various scenarios for the production of ethyl lactate.

- Case 1 High concentration of lactic acid

  Water content is low, but the oligomer lactic acids is high. It means production process does not need a lot of energy to separate the substance. On the other hand, the percentage of the product yield will decrease.

- Case 2 Low concentration of lactic acid

  Water content is high, but the oligomer lactic acids is low. The higher water content in the lactic acid solution results in higher energy requirements to separate the product. Conversely, the percentage of product yield increases as the quantity of the oligomer lactic acid decreases.

Process design and simulation are followed by two ethyl lactate productions at different lactic concentrations, and an economic analysis is performed to choose the suitable manufacturing process using reactive distillation.

1.2 Objective

The purpose of this project is to simulate ethyl lactate production via esterification of lactic acid and ethanol over Amberlyst-15 cation exchange resin catalyst with a reactive distillation method and to investigate the effect of lactic acid concentrations in feed stream on process performance and economic. Eventually, the simulation results will be compared to indicate the proper scenarios.

1.3 Scope of work

1.3.1 Ethanol and lactic acid derived from biomass are used as reactants.

1.3.2 The main reaction, esterification of ethanol and lactic acid, occurs in Amberlyst-15 cation exchange resin catalyst, which is packed in the reactive section of the reactive distillation column.

1.3.3 Various lactic acid concentration is dependent variable to simulate ethyl lactate production. The commercial lactic acid conditions in this project are as follows:

- Lactic acid solution 50 wt.% in water
- Lactic acid solution 85 wt.% in water

1.3.4 Aspen plus is used to simulate process design and Aspen economic analysis is used to evaluate economics.

1.3.5 Performance indexes to be used as a measure of the efficiency of the manufacturing process are economic, energy, and carbon dioxide emissions.

1.4 Expected benefits

To gain insights of the factors affecting the ethyl lactate production via esterification of ethanol and lactic acid using process simulation. Utilization of the simulator will facilitate the preliminary estimation of process efficiency, energy consumption, and profitability. The results of ethyl lactate process design and simulation will benefit the chemical industry and provide a new alternative to the more environmentally friendly production of the green solvent.

CHAPTER II
FUNDAMENTALS AND LITERATURE REVIEWS

The provided information relates to lactic acid, ethanol, ethyl lactate, esterification reaction, ethanol recovery method and input parameters for simulating the ethyl lactate production process.

2.1 Fundamental

2.1.1 Lactic acid

Lactic acid can be produced either by being synthesized from a chemical reaction or from the microbial fermentation process. Generally, lactic acid bacteria for the lactic acid fermentation process are recognized as safe microorganisms, which are used for the preservation of food and various fermented food products. Therefore, the lactic acid from the fermentation is safe for use in various fields.[5]

Currently, biobased lactic acid is used as raw material to produce new chemical products. The chemical routes of the biobased lactic acid are shown in Figure 1.

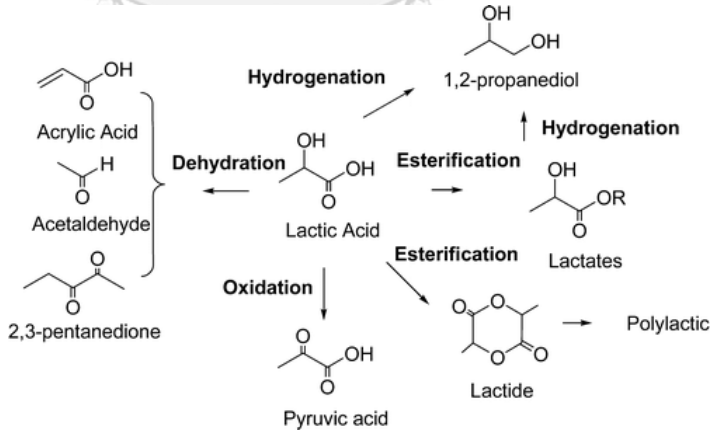


Figure 1. Chemical produced from lactic acid.[5]

The lactic acid in aqueous solution has a behavior known as oligomerization of the two molecules of lactic acid. When the lactic acid concentration is higher than 30 wt.%, the monomer lactic acid will undergo the oligomerization reaction, transforming the monomer into oligomer acids. Therefore, the content of lactic acid that is required for the esterification process is reduced by the existence of the oligomer acids.

2.1.2 Ethanol

Ethanol, one of the key components in the chemical industry, can be derived from biomass materials such as wood, crops, sugar, etc. Ethanol can be used as fuel in transportation which helps reduce harmful greenhouse gas compared to petroleum fuel. Ethanol usage is not only used as fuel, but it is also used to produce chemicals as illustrated in Figure 3.

Figure 3 shows the versatility transformation of ethanol as a fundamental chemical into valuable products such as ethylene, acetaldehyde, ethyl acetate, etc.

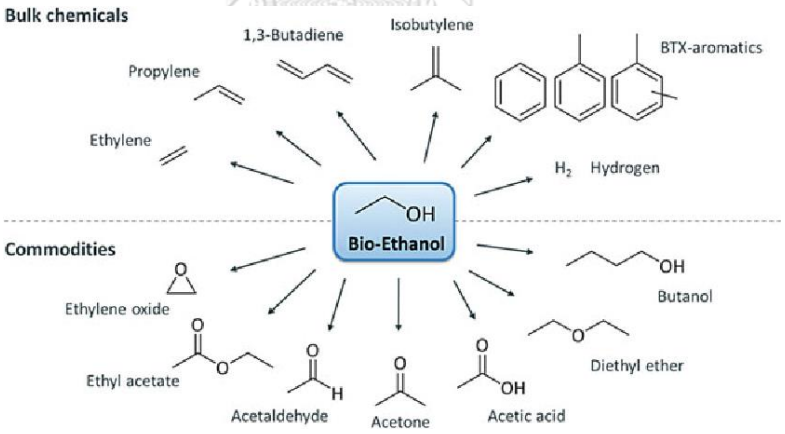


Figure 2. Example of chemicals produced from ethanol.[6]

2.1.3 Ethyl lactate

Solvent is one of the key components in the chemical industry. Ethyl lactate can replace up to 80% of the solvent used, currently. The appearance of ethyl lactate is slightly yellow liquid with the characteristic odor. The basic properties of ethyl lactate are shown in table 1.[7, 8]

Table 1. Physical and chemical properties of ethyl lactate

Properties	Unit	Value
Appearance	-	Colorless
Odor	-	Mild characteristic
Melting point	℃	-26
Boiling point	℃	154
Density at 25 ℃	g mL^{-1}	1.031
Refractive index	-	1.4124
Flash point	℃	54.6±6.4
Solubility	-	Miscible with water

Both lactic acid and ethanol can be synthesized from biomass fermentation. Esterification reaction between ethanol and lactic acid is one of the conventional methods to produce ethyl lactate. There are two-phase types of acid catalyst for the esterification of lactic acid with ethanol: liquid and solid phase. The common liquid and solid acid catalysts are sulfuric acid and Amberlyst 15, respectively. The common type of catalyst for esterification of lactic acid with ethanol is liquid acid catalyst.

Table 2. An ethyl lactate production comparison between esterification of lactic acid with ethanol over sulfuric acid and Amberlyst-15 catalyst.[9]

List	Sulfuric acid (Liquid catalyst)	Amberlyst-15 (Solid catalyst)
Not affected by water content in feedstock	✓	✓
Simultaneous esterification	✓	✓
Easy separation of catalyst from product	✗	✓
Possibility to reuse and regenerate catalyst	✗	✓
Non-necessity for catalyst neutralization	✗	✓
Non-necessity of a stage for catalyst removal	✗	✓
Environmentally friendly	✗	✓
Less piping corrosion	✗	✓

*When green color is good and red color is not good.

As shown in Table 2, ethyl lactate production via esterification of lactic acid with ethanol over Amberlyst-15 acid catalyst can act as a catalyst as well as sulfuric acid catalyst. Moreover, The Amberlyst-15 acid catalyst has advantages over sulfuric acid catalyst in terms of easy to separate, reusable, and environmentally friendly. Therefore, in this project, the esterification of lactic acid with ethanol over Amberlyst-15 is selected.

2.2 Literature reviews

This section, a review of the literatures on ethyl lactate production via esterification of lactic acid and ethanol, is divided to 3 main topics: experiment data for ethyl lactate production, strategy for ethanol recovery, and oligomer distribution in lactic acid.

2.2.1 Experiment data for ethyl lactate production via esterification of ethanol and lactic acid

Miller et al. (2010) studied organic acid esters production using reactive distillation column packed with the acid catalyst.

The reactive distillation column is different from the normal distillation column in that it doesn't have only the function used to separate the substance, but it also has a function of the reaction. As seen in Figure 3, the reactive distillation column has 3 partitions: rectifying, reactive, and stripping section.[10]

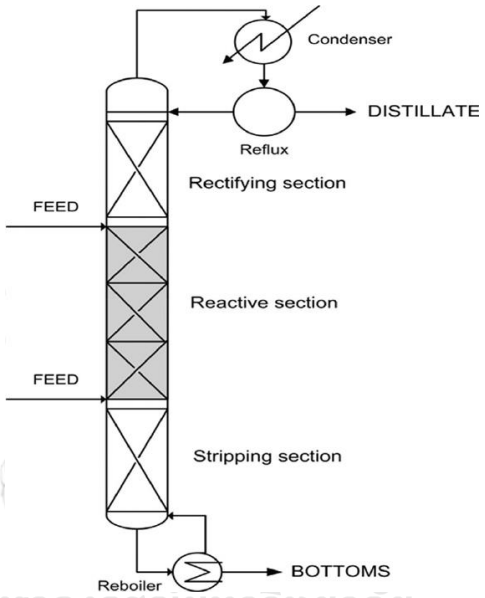


Figure 3. Diagram of reactive distillation column.[10]

The production of ethyl lactate through the esterification of lactic acid with ethanol was the subject of a study conducted by Miller et al. (2010) using a pilot-scale setup. The feed streams of ambient lactic acid solution and absolute ethanol were introduced at the top and bottom of the column, respectively. The reflux ratio was fixed at zero. The reactive zone, located between the top and bottom feed points, was where ethyl lactate was formed. The ethanol used in the experiment was of absolute purity. The experimental data for ethyl lactate formation is presented in Table 3.

Table 3. Experiment result of ethyl lactate formation in pilot-scale.[11]

Scenario	Ex.	LA feed composition	EtOH feed temperature	EtOH:LA	LA conversion	Yield
		Wt.%	℃	-	%	%
1	33	50	25	7.14	56.84	67.33
2	36	50	85	7.14	94.82	71.87
3	19	85	25	3.60	95.52	112.44
4	23	85	85	3.60	94.93	96.53

LA = Lactic acid

EtOH = Ethanol

EtLa = Ethyl lactate

L = Liquid recycled to the column

D = Distillate product

Comp. = Composition

Conv. = Conversion

Temp. = Temperature

Yield = Ethyl lactate yield based on monomer lactic acid in feed

C = Oligomers of lactic acid and ethyl esters

In addition, the experimental results were used as input data to simulate with ASPENPLUS™ software. The experiment number 33, 36, and 19 are recalled as Scenario 1, 2, and 3, respectively. The simulation was established based on a commercial-scale of ethyl lactate production at 25 million pounds per year using the simulation parameter from the experiment. The height of an equivalent theoretical plate (HETP) of 0.6 meters was used as a theoretical height of the packed column. Pure ethanol was fed in the reaction. Lactic acid monomer was used as a limiting reagent.[11] The simulation configurations and simulation results of the commercial scale are shown in Tables 4.

Table 4. Simulation configurations of commercial-scale ethyl lactate production [11].

Column configuration	Unit	Ethyl lactate production (Ethanol + Lactic acid)
Number of stages	-	40
Feed location	-	2 and 35
Reactive stages	-	7 to 35
Reflux ratio	-	0.001
Boil-up ratio	-	5
Column height	Meter	22
Column diameter	Meter	1

2.2.2 Operation strategy for separation of ethanol-water by extractive distillation

According to a high ratio of ethanol to lactic acid from Table 3, this can result in the excess of ethanol remaining from the ethyl lactate production. Therefore, the recovery of ethanol residue was important for cost reduction. The ethanol leftover from esterification was mixed with water. Generally, a distillation tower is used first to separate ethanol and water. The purity of ethanol from the distillation column was limited by the azeotrope point of ethanol and water. The ethanol-water mixture forms a minimum boiling azeotrope of 89.4 mol% ethanol.

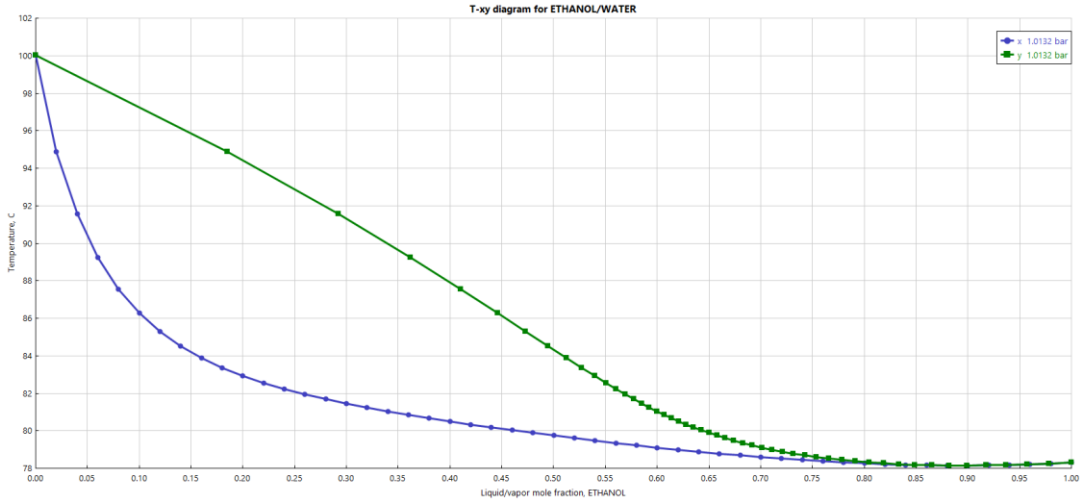


Figure 4. Binary x-y diagram of ethanol-water mixture using NRTL model.

So, the distilled ethanol was not yet pure enough to be recycled. The next step of ethanol purification can be mainly done with three popular methods: extractive distillation, pressure swing adsorption, and pervaporation membrane.[12]

From the comparison shown in Table 5, pressure swing adsorption and pervaporation membrane methods are more cost and energy efficient. However, they have been favorably used for ethanol recovery in laboratory scale. Thus, in industrial scale, ethanol purification is mostly done by extractive distillation.

Table 5. Advantage comparison of ethanol recovery method.[12]

Advantage comparison	Extractive distillation	Pressure swing adsorption	Pervaporation membrane
High separation capacity	✓	×	×
Simplicity of operation	✓	×	×
Easy for maintenance	✓	×	×
Low sensitivity	✓	×	×
Expert labor requirement	×	✓	✓
Energy efficient	×	✓	✓
Cost efficient	×	✓	✓
Industrial scale	✓	×	×

Guangzhong Li and Peng Bai studied the new operation strategy for extractive distillation to separate ethanol and water after distillation at the azeotrope point. They use ethylene glycol, which is a solvent for a typical extractive distillation column, to dehydrate ethanol. In this new operation strategy, there are 2 main columns, extractive distillation, and a solvent recovery column, and 1 optional column for purification water from the distillate stream of the solvent column to reduce waste emissions. The achievement of ethanol concentration in the extractive distillate reaches the composition specification at 99.95 mol%.[13] The configurations of the extractive distillation column are shown Table 6.

Table 6. Column configurations of the new operation strategy for ethanol recovery.[13]

Parameter	Unit	Extractive column	Recovery column	Concentrate column
Number of stages	-	25	12	25
Feed location	-	22	6	16
Solvent feed location	-	7		
Reflux ratio	-	0.1	0.5	3
Condenser	-	Total	Total	Total
Top stage pressure	atm	1	1	1
Solvent to feed mole ratio	-	1		

2.2.3 Oligomer distribution in lactic acid solutions

This section will add information on the raw materials. The form of lactic acid used in the esterification reaction with ethanol to produce ethyl lactate in Section 2.2.1 is monomer lactic acid, but the lactic acid solution does not contain only monomer lactic acid but also dimer, trimer, tetramer lactic acid, collectively referred to as lactic acid oligomer. The proportion of lactic acid oligomer is directly proportional to the concentration of lactic acid solution. The lactic acid content of each concentration can be found in Table 7. The superficial acid weight percent is indicated as the weight of total monomer divided by total solution weight. In this work, the superficial acid concentrations 50 and 85 are selected for ethyl lactate production via esterification of lactic acid and ethanol.[14]

Table 7. Lactic acid composition with total superficial acid by titration.[14]

Overall superficial wt.% LA%		HPLC analysis (%EMLA)					
Titration	HPLC	LA_1	LA_2	LA_3	LA_4	LA_5	LA_6
12.24	10.81	99.63	0.37	0.00	0.00	0.00	0.00
24.36	26.88	96.31	3.59	0.10	0.00	0.00	0.00
44.47	47.62	94.74	5.06	0.20	0.00	0.00	0.00
53.43	51.25	94.53	5.28	0.19	0.00	0.00	0.00
59.59	62.02	89.95	9.33	0.72	0.00	0.00	0.00
70.60	71.93	84.61	13.58	1.65	0.16	0.00	0.00
81.46	81.90	75.66	19.49	3.88	0.69	0.28	0.00
87.13	89.62	65.92	25.05	6.90	1.63	0.49	0.00
88.06	89.63	66.85	24.09	6.87	1.72	0.48	0.00
96.75	96.42	54.42	28.56	11.48	3.84	1.38	0.32

%EMLA = Percent of equivalent monomer lactic acid on a water free basis.

2.2.4 Novelty aspects of this work

Based on the literature review, there are couple points that required to be fulfilled. First, the form of lactic acid used in the literature review is a monomer lactic acid. However, in fact, besides the monomer lactic acid, there are also dimer, trimer, tetramer, etc. Second, the production processes mentioned in the literature review are only the reaction section, which is a subset of ethyl lactate production processes. Other important aspects of the ethyl lactate production process are ethanol recycling, ethyl lactate purification, etc.

In this work, the composition of lactic acid used to react with ethanol to produce ethyl lactate is shown in Table 7. and there will be an additional production process design to build on from Miller et al. (2010) in terms of production processes and product quality.

CHAPTER III

METHODOLOGY

This chapter discusses in detail the research methodology for simulation and economic analysis of ethyl lactate production via esterification of ethanol and lactic acid. There were 3 main parts: data collection, process simulation, and process economic. In step 1, data collected will consist of operating conditions, unit operations, reactions, and feed utilization. In step 2, the process simulation uses a program to simulate each scenario of production process. In last step, the comparison of the production process in each scenario will be conducted using a variety of economic evaluation tools, taking into consideration factors such as energy consumption and environmental impact, in order to assess the overall efficiency of the production process.

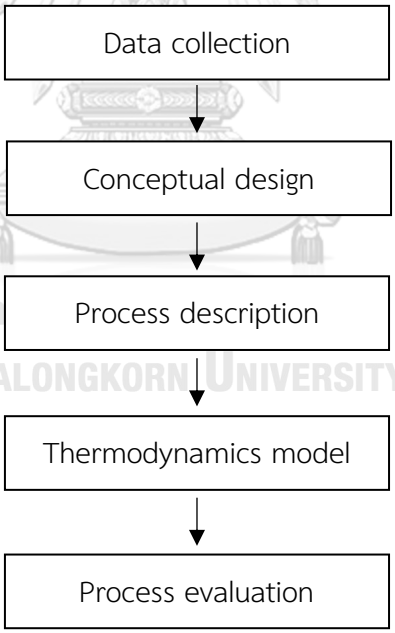


Figure 5. Research methodology routes

3.1 Data collection

The data collection process was segmented into two distinct categories: simulation data and reaction kinetics.

3.1.1 Simulation data

The production of ethyl lactate through the esterification of lactic acid with ethanol was the subject of a study conducted by Miller et al. (2010) using a pilot-scale setup. The feed streams of ambient lactic acid solution and absolute ethanol were introduced at the top and bottom of the column, respectively. The reflux ratio was fixed at zero. The reactive zone, located between the top and bottom feed points, was where ethyl lactate was formed. The ethanol used in the experiment was of absolute purity. The experimental data for ethyl lactate formation is presented in Table 3.[11]

In addition to the experimental results, they were utilized as input data for simulation utilizing ASPENPLUS software. The experiment number 33, 36, 19, and 23 are recalled as Scenario 1, 2, 3, and 4, respectively. The simulation was based on a commercial-scale ethyl lactate production of 25 million pounds per year, using parameters obtained from the experiment. The height of an equivalent theoretical plate (HETP) of 0.6 meters was employed as the theoretical height of the packed column. Absolute ethanol was utilized as the reactant feed. The limiting reagent was lactic acid monomer. The configuration of the simulation is presented in Table 4.[11]

The esterification reaction between ethanol and lactic acid to produce ethyl lactate utilizes monomer lactic acid, however, the lactic acid solution used in the reaction is not limited to monomeric form but also includes dimeric (L_2), trimeric (L_3), tetrameric (L_4) forms, collectively referred to as lactic acid oligomers. Due to the small quantity of L_3, L_4, L_5, and L_6 and limitations on the chemical components in the simulation program, they were combined into L_2 for ease of simulation. The composition of lactic acid is presented in Table 8.[14]

Table 8. Superficial acid concentrations of lactic acid at 50 and 85 wt.%.

Superficial	Superficial	True weight percent composition		
wt.% LA	wt.% H_2O	H_2O	L_1	L_2
50	50	50.4	46.3	3.30
85	15	17.5	62.2	20.3

3.1.2 Reaction kinetics

Typically, ethyl lactate is produced from esterification reaction of ethanol and lactic acid monomer (L_1). The catalytic esterification reaction is provided in the equation 1.

Main reaction:

$$L_1 + EtOH \rightleftharpoons L_1E + H_2O \quad (1)$$

Lactic acid in aqueous solution exhibits a behavior known as oligomerization or self-esterification of the two molecules of lactic acid. This reaction increases with increasing lactic acid concentration. The monomer lactic acid undergoes an oligomerization reaction, resulting in the formation of oligomer acids.[14] As a result, the amount of lactic acid required for the esterification process is reduced due to the presence of oligomer acids. The oligomerization reaction pathways are depicted in equations 2 and 3, while the esterification of oligomers is described in equations 4 and 5.

Lactic acid dimer (L_2) formation:

$$L_1 + L_1 \rightleftharpoons L_2 + H_2O \quad (2)$$

Lactic acid trimer (L_3) formation:

$$L_1 + L_2 \rightleftharpoons L_3 + H_2O \quad (3)$$

Ester of lactic acid dimer (L_2E) formation:

$$L_2 + EtOH \rightleftharpoons L_2E + H_2O \quad (4)$$

Ester of lactic acid trimer (L_3E) formation:

$$L_3 + EtOH \rightleftharpoons L_3E + H_2O \quad (5)$$

The compositions of lactic acid are presented in Table 3. With regards to the chemical reactions, only Equations 1, 2, and 4 are considered, as Equations 3 and 5 were omitted. The kinetic expressions for each component are presented in Equations 6-8.[15]

$$-\frac{dx_{L_1E}}{dt} = w_{cat}[k_1^0 exp(-\frac{E_{A_1}}{RT})(x_{L_1}x_{EtOH} - \frac{x_{L_1E}x_w}{K_1})] \quad (6)$$

$$-\frac{dx_{L_2E}}{dt} = w_{cat}[k_2^0 exp(-\frac{E_{A_2}}{RT})(x_{L_1}x_{EtOH} - \frac{x_{L_2E}x_w}{K_2})] \quad (7)$$

$$-\frac{dx_{L_2}}{dt} = w_{cat}[k_3^0 exp(-\frac{E_{A_3}}{RT})(x_{L_2}x_w - \frac{x_{L_1}^2}{K_3})] \quad (8)$$

The kinetic parameters, equilibrium constants (K_i), pre-exponential factors (k_i^0), and activation energies (E_{A_i}), of the simple nth-order reversible kinetic expression are described in Table 9.[15]

Table 9. Kinetic model parameters.

Parameter	Unit	Value
k_1^0	$kg_{sol}.K/kg_{cat}/s$	1.91×10^5
k_2^0	$kg_{sol}.K/kg_{cat}/s$	2.66×10^4
k_3^0	$kg_{sol}.K/kg_{cat}/s$	1.62×10^7
E_{A_1}	kJ/kmol	4.80×10^4
E_{A_2}	kJ/kmol	5.45×10^4
E_{A_3}	kJ/kmol	5.20×10^4
K_1	-	2.40
K_2	-	0.600
K_3	-	5.00

The kinetic parameters derived from the experimental results at a lactic acid concentration of 20 wt.% were subsequently utilized to predict the outcomes of ethyl lactate production at concentrations of 50 and 85 wt.%. The associated percentage errors, as depicted in the table 10, were used to assess the accuracy of the predictions.

Table 10. Comparison of experimental values and model prediction for esterification of 20, 50, and 88 wt.% lactic acid with ethanol.

EtOH:LA molar ratio	catalyst loading (wt.%)	reaction temp. (°C)	Percent Error							
			L_1	L_2	L_3	L_1E	L_2E	L_3E	EtOH	Water
88 wt.% Lactic acid solution										
1	3	80	8.7	19.9	24	20.5	37.1	25.1	10.9	5.2
2	3	80	8.9	17.2	15.5	10.1	15.9	25	4.4	2.3
3	3	80	13.9	15.8	11.2	7.7	12.2	20.5	2	2.1
4	3	80	22.2	21	12.8	2.7	16.9	25	1.1	0.9
3	1	80	11.3	9.8	9.3	11.2	16	31.2	1.6	2.1
3	2	80	7.4	10.1	7.6	7	9	29.8	1.4	1.6
3	4	80	15.7	7	4.8	3.6	5.7	29.1	1.4	1
3	5	80	11.5	33.4	27.9	2.6	6.6	16	1.2	0.6
3	3	62	8.3	1.2	1.8	2.5	9.6	31.5	0.8	0.8
3	3	72	5.5	3.5	3.2	0.6	3.6	13.1	0.6	0.2
3	3	90	9.5	41.8	25.9	6.6	14.5	29.6	3	4.2
50 wt.% Lactic acid solution										
1	3	80	2.6	6.9		20.2	49		6.2	0.4
2	3	80	2.2	5.1		11.2	29.2		2.9	0.04
3	3	80	5.1	10.3		4.8	37.1		1.1	0.4
4	3	80	8.4	20.4		5	25.9		0.5	0.6
3	1	80	4.2	1.8		13	14.7		2	0.2
3	2	80	5.6	6		4	24.4		1	0.4
3	4	80	6.3	14		3.5	24.7		1.4	0.4
3	3	62	6.6	3.2		14.2	39.1		0.4	0.8
3	3	72	7.1	8.4		5.2	14.8		1.2	0.6
3	3	90	1	20.8		4.1	34.8		1.2	0.5

EtOH:LA molar ratio	catalyst loading (wt.%)	reaction temp. (°C)	Percent Error							
			L_1	L_2	L_3	L_1E	L_2E	L_3E	EtOH	Water
20 wt.% Lactic acid solution										
1	3	80	1.5			9.2			0.8	0.06
2	3	80	1.4			3.5			0.3	0.05
3	3	80	1.8			4.2			0.2	0.07
4	3	80	4.4			17			0.1	0.2
3	1	80	5.8			9.7			1.3	0.4
3	2	80	1			5.8			0.2	0.03
3	4	80	2			14.1			0.7	0.2
3	3	60	1.2			2.8			0.2	0.08
3	3	70	2.5			5.6			0.5	0.2
3	3	90	1.2			4.6			0.2	0.05

The predictions generated for the component profiles demonstrated a high degree of consistency with the experimental findings obtained for the production of ethyl lactate using 20 wt.% lactic acid.

In the experiments involving 50 and 88 wt.% lactic acid concentrations, the errors observed were minimal. Notably, the errors were primarily concentrated in the concentration of oligomers and oligomer esters, which constitute a relatively small proportion of the overall components. Therefore, their impact on the concentration of the primary constituent was negligible.

In this project, simulation data will be from works of literature. Process configurations of ethyl lactate production process via lactic acid and ethanol over Amberlyst-15 cation exchange resin catalyst and ethanol recovery process are represented in Table 5 and Table 6, respectively. This work will focus on comparing process profitability, and energy consumption.

3.2 Conceptual design

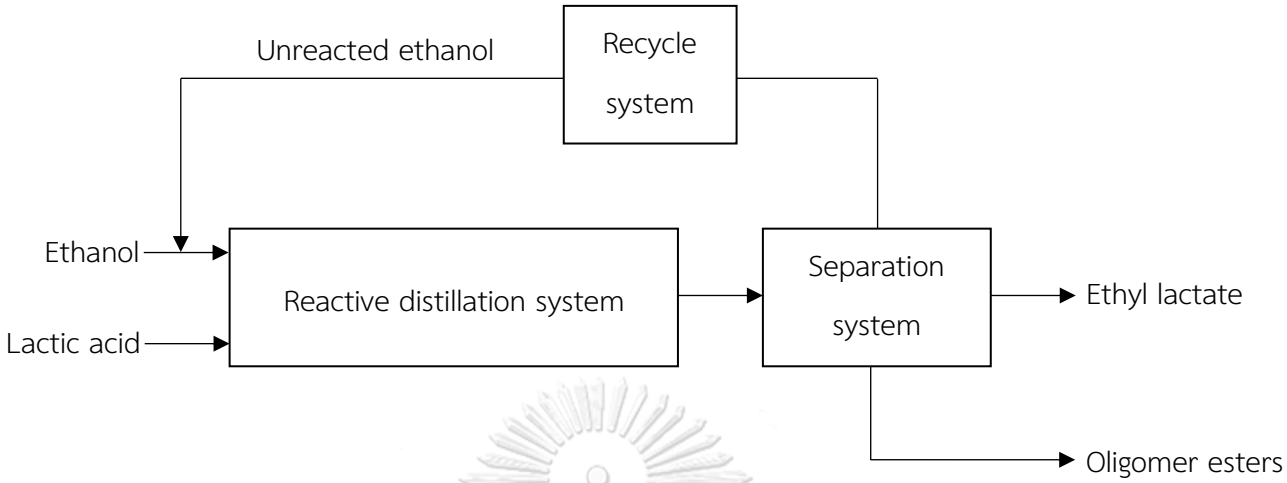


Figure 6. Block flow diagram of ethyl lactate production via esterification of ethanol and lactic acid.

The conceptual design represented in Figure 6. can be separated into 3 systems:

3.2.1 Reactive distillation system

Normally, the raw material conversion in the chemical process will occur in a reactor and classify the primary product with a separator. If the reaction is a liquid-liquid reaction, the separator would be a distillation column. So, the general design of liquid-liquid reaction in the chemical process requires a reactor followed by the distillation column. However, the conversion of raw material for reversible reactions is limited when the equilibrium is achieved. As mentioned above, reactive distillation is a new technique to combine both reaction and separation systems in one unit operation. The reactive distillation technique does not only increase the purity of the product but also reduces the capital cost such as pump cost, instrument cost, etc [10].

The esterification of ethanol and lactic acid to produce ethyl lactate is occurred in the reactive zone of the reactive distillation column. After the ethyl lactate is generated, it will be separated and sent out through a bottom stream. The operating pressure of the reactive distillation column is at a constant pressure of 1 atm.

3.2.2 Separation system

The main function of this system is to purify ethyl lactate and separate ethanol from ethanol-water mixtures for recovery ethanol to the reaction system. The main type of unit operation of the separation system is the distillation column. First, distillation column model “DSTWU” in Aspen plus will be used to calculate the initial estimations: feed location, number of stages, reflux ratio, and distillate rate. Four configuration variables from DSTWU will be applied to the distillation column model “RADFRAC” in Aspen plus. After that, a DesignSpec function of the RADFRAC is set for vary reflux ratio and distillate rate to get the desired product purity at 99.5 wt.%.

3.2.3 Recycle system

For esterification of ethanol and lactic acid occurs over Amberlyst-15 cation exchange resin catalyst packed in the reactive zone of the reactive distillation column, lactic acid is the limiting reagent. Ethanol is used more than enough to react with lactic acid. The unreacted ethanol from the separation system is recycled back to the reaction system.

3.3 Process description

The process flow diagram of ethyl lactate production process is illustrated in Figure 7. by using Aspen plus program.

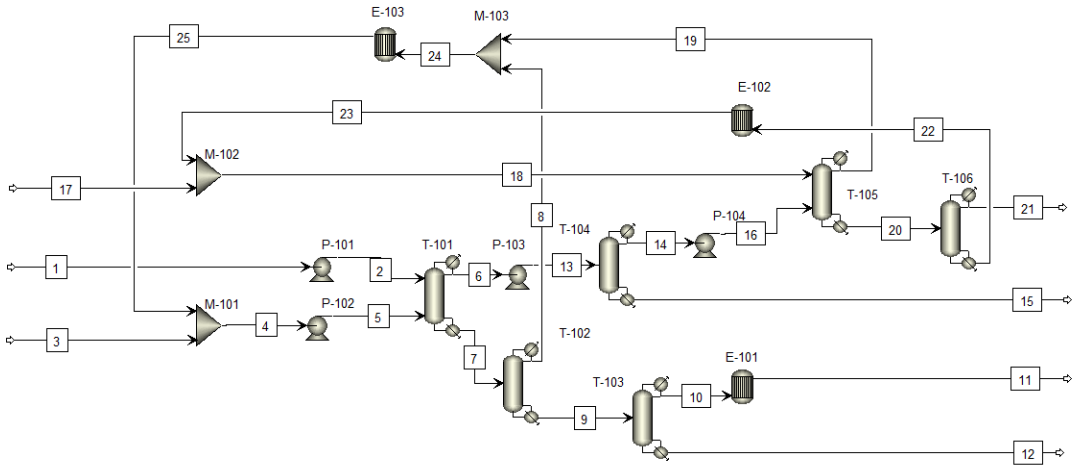


Figure 7. Process flow diagram of ethyl lactate production via esterification of ethanol and lactic acid for Scenario 1 and 3.

From process flow diagram in Fig. 1, 99.5 wt.% of fresh ethanol (Stream 3rd) is mixed with the unreacted ethanol (Stream 28th) in the mixer, M-101 and the unreacted lactic acid (Stream 18th), respectively. The mixed ethanol (Stream 4th) and the fresh lactic acid (Stream 1st) are fed to the reactive distillation column, T-101. Esterification reaction of ethanol and lactic acid is occurred over Amberlyst-15 cation exchange resin catalyst packed in the reactive section of the reactive distillation column to produce the primary product, ethyl lactate. The outlet stream of T-101 is stream 8th, mixtures of ethyl lactate, oligomer esters, and ethanol. The ethanol in stream 7th is separated with a distillation column, T-102, as a distillate stream. The bottom stream of T-102 (Stream 9th) is sent to the distillation column, T-103, to purify ethyl lactate to a concentration of 99.9 wt.% (Stream 10th) and adjust temperature to 35 ℃ with the heat exchangers, E-101, for storage (Stream 11th).

Ethanol-water mixtures (Stream 6th) from T-101 are transfer to the distillation column, T-104, to recover ethanol. Majority of ethanol and water are separated to

the stream 14th and 15th, respectively. 90 wt.% ethanol from stream 14th is sent to the ethanol purification system. T-105, an extractive distillation column, is used to purify ethanol from 90 to 99.5 wt.% by using ethylene glycol as a solvent (Stream 17th). Ethylene glycol is recycled with a distillation column, T-106. The unreacted ethanol at 99.5 wt.% is adjusted operating temperature to 35 °C with heat exchangers, E-102, and recycled back to the process (Stream 23rd).

The process diagram in Fig. 1 can apply with Scenarios 1 and 3. For Scenario 2, the feed ethanol was in the vapor phase at 85 °C. Therefore, there must be two additional unit operations, a preheater and a compressor before being sent to react with the lactic acid at the reactive distillation, T-101.

The process diagram in Fig. 7 can apply with Scenarios 1 and 3. The process diagram of Scenario 2 is shown in Fig. 8. For Scenario 2, the feed ethanol was in the vapor phase at 85 °C. Therefore, there must be two additional unit operations, a preheater and a compressor before being sent to react with the lactic acid at the reactive distillation, T-101.

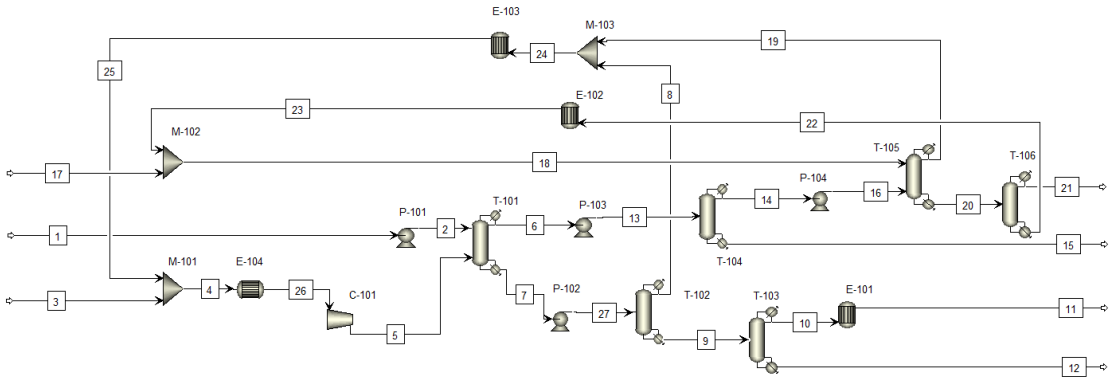


Figure 8. Process flow diagram of ethyl lactate production via esterification of ethanol and lactic acid for Scenario 2.

3.4 Thermodynamics model used

The operating conditions of ethyl lactate production process is at low pressure, see more detail in Table 6. According to Thermodynamics model selection guideline [16], there are polar components and binary azeotrope between ethanol and

water. Thus, the activity coefficient thermodynamic model (NRTL) is appropriate to express the ethyl lactate production process.

3.5 Process evaluation

3.5.1 Economic analysis

In process evaluation, the initial cost estimation will be conducted utilizing the Aspen Plus Economic Analyzer (APEA). The costs associated with the production of ethyl lactate are presented in Table 11.

Table 11. Chemical cost for ethyl lactate production.

Component	Unit	Value
Ethanol [17]	US$/L	0.58
Lactic acid at 50 wt.% [18]	US$/kg	1.00
Lactic acid at 85 wt.% [18]	US$/kg	1.90
Ethyl lactate [19]	US$/kg	3.50
Ethylene glycol [20]	US$/kg	0.71

Investment decisions should not be based solely on the Net Present Value (NPV), but should also take into account other factors such as the Payout Period (POP) and the Internal Rate of Return (IRR). The Payback Period provides insight into the duration of the investment during which the net cash inflows from the project are equal to the net cash outflows. The Internal Rate of Return (IRR) serves as an indicator of the return on a project in relation to the minimum return required or the set capital value.

3.5.2 Energy consumption

Specific energy consumption (SEC) is an important factor to evaluate process performance. SEC can be calculated by the following equation.

$$\text{Specific energy consumption (SEC)} = \frac{\text{Energy consumption}}{\text{Product amount}} \quad (9)$$

In this work, the price list of utilities used to calculate the energy consumption is shown in Table 12.

Table 12. Utilities price.[21]

Utility	Unit	Value
Cooling water	US$/ton	0.015
Refrigerated water	US$/ton	0.185
Electricity	US$/kWh	0.06
Natural gas	US$/GJ	11.10
Low pressure steam	US$/ton	29.29
Medium pressure steam	US$/ton	29.59
High pressure steam	US$/ton	29.97

3.5.3 Carbon dioxide emissions

In terms of environmental impact, the widespread implementation of projects aimed at reducing greenhouse gas emissions has become increasingly necessary due to the rising levels of carbon dioxide in the atmosphere. Energy consumption plays a significant role in carbon dioxide emissions. Carbon dioxide emissions can be calculated by analyzing the amount of energy consumed and wastewater treatment. The carbon dioxide equivalent emissions factors are described in Table 13.[22]

Table 13. Carbon dioxide emissions factors.

Index	Unit	Value
Electricity	kg $CO_{2\text{-eq}}$/kWhr	0.67
Wastewater	kg CO_2-eq/kg COD removed	1

CHAPTER IV
RESULT AND DISCUSSION

This chapter provides a comprehensive exposition and analysis of the results obtained from the study. It is organized into four major sections, each of which is dedicated to a specific aspect of the research. These sections include a detailed of the simulated results of ethyl lactate production, an economic analysis, an assessment of energy consumption, and an evaluation of carbon dioxide emissions.

4.1 Raw material utilization

Table 14 provides conversion and yield of esterification of ethanol and lactic acid between a reactive distillation column and an equilibrium reactor. The esterification process of lactic acid with ethanol is accomplished in a reactive distillation column, wherein two distinct ethanol streams - namely, fresh feed and recycle streams - are utilized. The simulation results indicate a conversion rate of 74.3%, 81.5%, 87.9%, and 81.3% for Scenarios 1, 2, 3, and 4, respectively. In instances where the process operates with an excessive amount of ethanol, ethanol recovery becomes necessary. Accordingly, the yield rates for Scenarios 1, 2, 3, and 4 are 90.6%, 80.2%, 128%, and 119%, respectively.

In terms of comparing the conversion and yield of ethyl lactate production between a reactive distillation column and a continuous stirred tank reactor, utilizing the same liquid holdup and fixed production capacity of 6,200 kg/hr, the reactive distillation column exhibits markedly superior conversions and yields in comparison to the continuous stirred tank reactor. The reactive distillation column, which integrates the separation and reaction units, consistently results in the separation of reactants, thereby facilitating a forward shift in the reaction equilibrium.

For the yield of the continuous stirred tank reactor method, a portion of the lactic acid oligomers undergo reverse reaction, leading to the formation of lactic acid monomers. This phenomenon results in a molar ratio of the product formed in excess of 100 relative to the amount of lactic acid monomer utilized.

Table 14. Comparison of conversion and yield of a reactive distillation column and an equilibrium reactor.

Scenario	Liquid holdup	Reactive distillation column		Continuous stirred tank reactor	
		Conversion	Yield*	Conversion	Yield*
	m^3	%	%	%	%
1	38.5	74.3	90.6	1.44	114
2	42.8	81.5	80.2	1.60	114
3	26.7	87.9	128	1.56	294
4	20.4	81.3	119	1.14	309

*Yield is the amount of a specific product formed per mole of reactant consumed.

4.2 Simulated results of ethyl lactate production

As detailed in Chapter 3, Section 3.3, the process flow diagrams demonstrate the stream results obtained from the production of ethyl lactate under different operating conditions. Specifically, Table 15 outline the results of Scenario 3, which boasts the highest conversion and yield. However, for alternative capacities, stream results can be found in Appendix B.

Table 15. Stream results of ethyl lactate production of Scenario 3.

Parameter	Units	Stream no.						
		1	2	3	4	5	6	7
Temperature	°C	35.0	35.0	35.0	35.0	35.0	79.5	166
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.00	1.34
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	122	122	60.1	171	171	231	61.6
Mass Flows	kg/hr	6.82×10^3	6.82×10^3	2.75×10^3	7.84×10^3	7.84×10^3	7.43×10^3	7.22×10^3
Ethanol	kg/hr	0.00	0.00	2.73×10^3	7.81×10^3	7.81×10^3	5.34×10^3	18.0
Water	kg/hr	1.19×10^3	1.19×10^3	13.7	22.2	22.2	2.07×10^3	0.170
L_1	kg/hr	4.24×10^3	4.24×10^3	0.00	0.00	0.00	17.2	496
L_1E	kg/hr	0.00	0.00	0.00	6.25	6.25	0.0800	6.25×10^3
L_2	kg/hr	1.38×10^3	1.38×10^3	0.00	0.00	0.00	0.640	417
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	38.7
Ethylene glycol	kg/hr	0.00	0.00	0.00	0.260	0.260	0.00	0.260

Table 15. Stream results of ethyl lactate production of Scenario 3. (Cont'd)

Parameter	Units	Stream no.						
		8	9	10	11	12	13	14
Temperature	°C	80.8	169	154	35.0	234	79.5	78.0
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	0.450	61.2	52.8	52.8	8.34	231	139
Mass Flows	kg/hr	24.4	7.20×10^3	6.24×10^3	6.24×10^3	958	7.43×10^3	5.60×10^3
Ethanol	kg/hr	17.99	0.00	0.00	0.00	0.00	5.34×10^3	5.08×10^3
Water	kg/hr	0.170	0.00	0.00	0.00	0.00	2.07×10^3	517
L_1	kg/hr	0.00	496	0.500	0.500	496	17.2	0.00
L_1E	kg/hr	6.25	6.24×10^3	6.24×10^3	6.24×10^3	6.25	0.0800	0.00
L_2	kg/hr	0.00	417	0.00	0.00	417	0.64	0.00
L_2E	kg/hr	0.00	38.7	0.00	0.00	38.7	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.26	0.01	0.01	0.24	0.00	0.00

Table 15. Stream results of ethyl lactate production of Scenario 3. (Cont'd)

Parameter	Units	Stream no.						
		15	16	17	18	19	20	21
Temperature	°C	96.5	78.0	35.0	35.0	78.0	158	96.8
Pressure	bar	1.34	1.34	1.34	1.34	1.00	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	92.1	139	1.38	137	110	166	30.0
Mass Flows	kg/hr	1.84×10^3	5.60×10^3	85.3	8.50×10^3	5.07×10^3	9.03×10^3	614
Ethanol	kg/hr	267	5.08×10^3	0.00	0.00	5.06×10^3	20.3	20.3
Water	kg/hr	1.55×10^3	517	0.09	5.22	8.27	514	509
L_1	kg/hr	17.2	0.00	0.00	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.0800	0.00	0.00	0.00	0.00	0.00	0.00
L_2	kg/hr	0.640	0.00	0.00	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.00	85.2	8.49×10^3	0.260	8.49×10^3	84.9

Table 15. Stream results of ethyl lactate production of Scenario 3. (Cont'd)

Parameter	Units	Stream no.			
		22	23	24	25
Temperature	°C	206	35.0	78.0	35.0
Pressure	bar	1.34	1.34	1.00	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	136	136	111	111
Mass Flows	kg/hr	8.41×10^3	8.41×10^3	5.09×10^3	5.09×10^3
Ethanol	kg/hr	0.00	0.00	5.08×10^3	5.08×10^3
Water	kg/hr	5.14	5.14	8.44	8.44
L_1	kg/hr	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.00	0.00	6.25	6.25
L_2	kg/hr	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	8.41×10^3	8.41×10^3	0.260	0.260

4.3 Economic analysis

This study presents a comprehensive techno-economic analysis of ethyl lactate production processes, utilizing Aspen Economic Analyzer software and adopting a fixed 10-year project timeline. To conduct the economic evaluation, we have established four production scenarios, while taking into account the reference prices for both chemicals and utilities, as outlined in Tables 5 and 10, respectively. Our findings demonstrate that, based on these reference prices, all ethyl lactate production scenarios are economically viable and profitable throughout the 10-year project timeline.

Utilizing the advanced Aspen Economic Analyzer software, we conducted an analysis of the esterification process of lactic acid and ethanol at varying concentrations of lactic acid. Specifically, Scenarios 1 and 2 involved the feeding of 50 wt.% of lactic acid, whereas Scenarios 3 and 4 utilized a feed of lactic acid at 85 wt.%. Our comprehensive economic evaluation of this process is presented in Table 16.

Table 16. Net present value (NPV), Internal rate of return (IRR), and Payout period (POP) at different production scenarios of ethyl lactate.

Items	Units	Scenario			
		1	2	3	4
Net present value	USD	7.82×10^6	2.48×10^7	1.76×10^8	7.72×10^7
Internal rate of return	%	21.3	24.1	74.6	37.9
Payout period	y	17.2	13.2	3.41	6.79

As appeared in the table, although Scenarios 1 and 2 have fewer raw material impurities than Scenarios 3 and 4, they are not economically advantageous. Because the high use of excess ethanol resulted in high operating costs for Scenarios 1 and 2. The economic result of ethyl lactate production process of Scenario 3 at lactic acid composition of 85 wt.% and ethanol feed temperature of 25 °C gives the good economic value with a NPV of 1.76×10^8 USD, IRR of 74.6%, and POP of 3.41 years.

4.4 Energy consumption

The primary energy-intensive unit operation in this production process comprises of two parts: the heat exchanger and the distillation column. The energy consumption of each equipment is presented and compared in Figure 9. As per Figure 1, the T-101 and T-104 distillation columns are the devices that consume the most energy, averaging at 60% of the total energy consumption in the production process. The T-101 distillation column is a reactive distillation device and is the primary unit operation in the production of ethyl lactate. It has a high initial substance content, leading to high energy consumption. The T-104 distillation column, on the other hand, separates ethanol from water. The substances fed into this unit operation include residual ethanol from the reaction, initial substance water, and water generated from the reaction. Due to the excessive use of ethanol in the reaction, the quantity of ethanol and water entering the T-104 distillation column is large, resulting in significant energy consumption for separation.

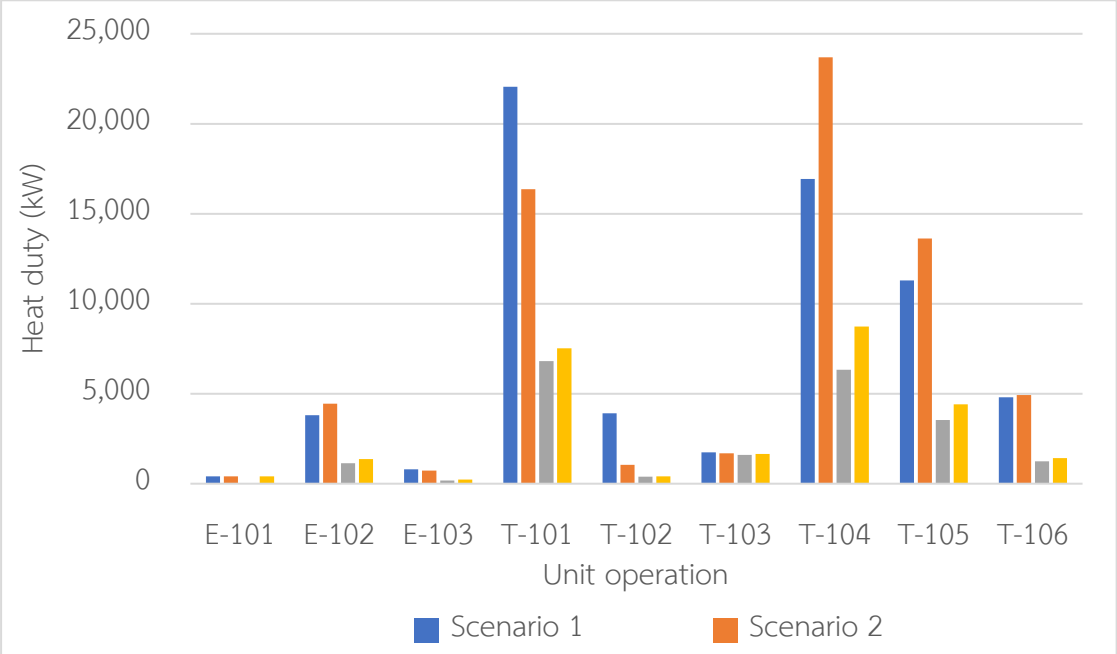


Figure 9. Research methodology routes

The energy consumption within the studied process can be broadly classified into two categories: electrical and thermal utilities. We have tabulated the respective quantities of these utilities for each scenario in Table 17.

Table 17. Summary of energy consumption.

Items	Units	Scenario			
		1	2	3	4
Total heating duty	kW	1.94×10^4	3.19×10^4	8.49×10^3	1.20×10^4
Total cooling duty	kW	2.70×10^4	2.92×10^4	7.70×10^3	9.34×10^3
L1E production	kg L_1E/h	6.24×10^3	6.24×10^3	6.24×10^3	6.20×10^3
SEC	kWh/kg L_1E	7.43	9.82	2.60	3.45

Moreover, the assessment of energy efficiency has been carried out by computing the specific energy consumption (SEC), which is the ratio of total electricity consumed to the total amount of ethyl lactate generated. Based on the SEC values obtained for Scenarios 1, 2, 3, and 4, which are 7.43, 9.82, 2.60, and 3.45 kWh/kg product, respectively, it can be inferred that Scenario 3 demonstrates the highest energy efficiency as it utilizes the least amount of energy.

4.5 Carbon dioxide emissions assessment

The total amounts of equivalent CO_2 released from the process are mainly obtained from electricity, process utilities, and waste treatment. Table 18 shows the amount of CO_2 generated in each production capacity of ethyl lactate.

Table 18. Equivalent carbon dioxide emissions

Type	Units	Scenario			
		1	2	3	4
Electricity	kg CO_2/year	2.31×10^8	3.06×10^8	8.08×10^7	1.07×10^8
Waste treatment	kg CO_2/year	4.28×10^7	4.25×10^7	1.46×10^7	2.40×10^7
Product production	kg L_1E/h	6,240.39	6,239.09	6,239.08	6,203.56
Total CO_2 emissions	kg CO_2/kg L_1E	5.49	6.97	1.91	2.63

The low concentration of lactic acid in the Scenario 1 and 2 that contributes to the increased amount of excess ethanol and waste. The excess ethanol requires a lot of energy to separate the ethanol from the product in any distillation columns and to recovery unreacted ethanol. For Scenarios 3 and 4, Scenario 4 has an increase in the energy consumption of additional unit operations entering the production process for ethanol phase change from liquid to vapor, thus resulting in higher carbon dioxide emissions than Scenario 3.

CHAPTER V
CONCLUSION

Biosolvents are gaining increasing importance in the chemical industry as they provide a more sustainable and environmentally friendly alternative to traditional solvents. Ethyl lactate, one of the biosolvents, is a versatile and sustainable solvent that offers several benefits to the chemical industry such as low toxicity, biodegradability, high solvency power, renewable resource, etc. Therefore, in this work, the utilization of lactic acid and ethanol to produce ethyl lactate via esterification of lactic acid and ethanol is processed due to the many benefits of acetaldehyde and its higher price.

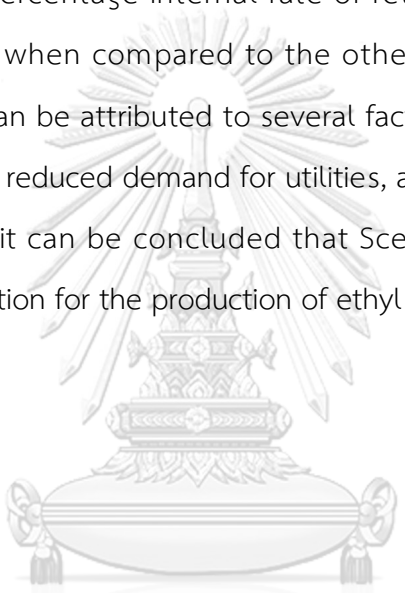
In this work, the process simulation and economic analysis of ethyl lactate production is conducted by Aspen Plus and Aspen Economic Analyzer, respectively. The experiment results obtained from published literatures regarding esterification of lactic acid with ethanol using Amberlyst-15 as the catalyst at different concentration of lactic acid and ethanol feed temperature. The simulation is divided into four scenarios according to the conditions.

Based on the analysis conducted at the same production capacity of ethyl lactate, it can be inferred that Scenario 3, operating at a lactic acid concentration of 85 wt.% and a temperature of 25 °C, represents the optimal condition. This conclusion is drawn from the observation that Scenario 3 delivers the highest percentage internal rate of return (%IRR), while concurrently exhibiting the lowest energy consumption and carbon dioxide emissions, thereby highlighting its superior economic and environmental performance.

With regard to the energy requirements, it was observed that the processes conducted in Scenarios 2 and 4 entail the utilization of significant quantities of electric utilities, owing to the addition of a heat exchanger and a gas compressor into the process. On the other hand, the processes implemented in Scenarios 1 and 2 involve the consumption of substantial amounts of thermal utilities, primarily due to

the entry of a large amount of ethanol into the process, necessitating the recycling of the increased amount of unreacted ethanol. Consequently, a significant thermal utility load is imposed on the process.

In determining the most suitable scenario for synthesizing ethyl lactate from lactic acid and ethanol, it was found that the optimal conditions involve producing acetaldehyde at an 85 wt.% concentration of lactic acid and a feed temperature of 25 °C for ethanol. This conclusion is based on the observation that this scenario delivers the highest percentage internal rate of return (%IRR) and the shortest payback period (POP) when compared to the other scenarios. These favorable economic outcomes can be attributed to several factors, including a lower excess ethanol requirement, a reduced demand for utilities, and lower equipment costs for the process. As such, it can be concluded that Scenario 3 represents the most economically viable option for the production of ethyl lactate.



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APPENDIX

APPENDIX A FEEDSTOCK ESTIMATION

This work involves simulating the process of producing ethyl lactate through esterification of lactic acid with ethanol over Amberlyst-15 catalyst using varying concentrations of lactic acid. The resulting data obtained from this experimental reaction is presented in Table A1, in accordance with established conventions.

Table A1. Conversion and yield in esterification of lactic acid with ethanol via reactive distillation column.

Scenario	LA feed comp.	EtOH feed Temp.	LA feed rate	EtOH feed rate	EtOH feed recycle	LA Conv.	Yield
	wt.%.	°C	kg/h	kg/h	kg/h	%	%
1	50	25	15,293.41	3,370.13	22,572.62	74.34	67.34
2	50	85	14,324.15	3,568.64	20,715.59	81.46	71.88
3	85	25	6816.04	2,746.26	5,090.85	87.88	112.44
4	85	85	7,893.92	2,804.68	6,318.07	81.28	96.54

APPENDIX B STREAM RESULTS

Table C1. Stream results of ethyl lactate production of Scenario 1.

Parameters	Units	Stream no.						
		1	2	3	4	5	6	7
Temperature	°C	35.0	35.0	35.0	35.0	35.0	80.0	96.4
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.00	1.34
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	510	510	73.7	566	566	854	221
Mass Flows	kg/hr	1.53×10^4	1.53×10^4	3.37×10^3	2.59×10^4	2.59×10^4	2.57×10^4	1.55×10^4
Ethanol	kg/hr	0.00	0.00	3.35×10^3	2.59×10^4	2.59×10^4	1.69×10^4	6.48×10^3
Water	kg/hr	7.71×10^3	7.71×10^3	16.8	77.1	77.1	8.76×10^3	25.2
L_1	kg/hr	7.08×10^3	7.08×10^3	0.00	0.00	0.00	23.0	1.79×10^3
L_1E	kg/hr	0.00	0.00	0.00	6.25	6.25	0.0500	6.25×10^3
L_2	kg/hr	505	505	0.00	0.00	0.00	0.220	939
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	18.6
Ethylene glycol	kg/hr	0.00	0.00	0.00	0.770	0.770	0.00	0.770

Table C1. Stream results of ethyl lactate production of Scenario 1 (Cont'd)

Parameters	Units	Stream no.						
		8	9	10	11	12	13	14
Temperature	°C	78	177	154	35.0	232	80.0	78.2
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	142	78.7	52.9	52.9	25.8	854	471
Mass Flows	kg/hr	6.51×10^3	9.00×10^3	6.24×10^3	6.24×10^3	2.76×10^3	2.57×10^4	1.83×10^4
Ethanol	kg/hr	6.48×10^3	1.38	1.38	1.38	0.00	1.69×10^4	1.61×10^4
Water	kg/hr	25.15	0.03	0.03	0.03	0.00	$8{,}76 \times 10^3$	2.19×10^3
L_1	kg/hr	0.00	1.79×10^3	1.79	1.79	1.79×10^3	23.0	0.00
L_1E	kg/hr	6.25	6.25×10^3	6.24×10^3	6.24×10^3	6.25	0.0500	0.00
L_2	kg/hr	0.00	939	0.00	0.00	939	0.220	0.00
L_2E	kg/hr	0.00	18.6	0.00	0.00	18.6	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.770	0.0100	0.0100	0.760	0.00	0.00

Table C1. Stream results of ethyl lactate production of Scenario 1 (Cont'd)

Parameters	Units	Stream no.						
		15	16	17	18	19	20	21
Temperature	°C	98.1	78.2	35.0	35.0	78	153	97.4
Pressure	bar	1.34	1.34	1.34	1.34	1.00	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	384	471	4.61	460	350	581	126
Mass Flows	kg/hr	7.44×10^3	1.83×10^4	286	2.85×10^4	1.61×10^4	3.07×10^4	2.50×10^3
Ethanol	kg/hr	847	1.61×10^4	0.00	0.00	1.60×10^4	64.4	64.4
Water	kg/hr	6.57×10^3	2.19×10^3	0.290	22.1	35.1	2.18×10^3	2.16×10^3
L_1	kg/hr	23.0	0.00	0.00	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.0500	0.00	0.00	0.00	0.00	0.00	0.00
L_2	kg/hr	0.220	0.00	0.00	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.00	285	2.85×10^4	0.770	2.85×10^4	285

Table C1. Stream results of ethyl lactate production of Scenario 1 (Cont'd)

Parameters	Units	Stream no.			
		22	23	24	25
Temperature	°C	206	35.0	78.0	35.0
Pressure	bar	1.34	1.34	1.00	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	455	455	492	492
Mass Flows	kg/hr	2.82×10^4	2.82×10^4	2.26×10^4	2.26×10^4
Ethanol	kg/hr	0.00	0.00	2.25×10^4	2.25×10^4
Water	kg/hr	21.8	21.8	60.2	60.2
L_1	kg/hr	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.00	0.00	6.25	6.25
L_2	kg/hr	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	2.82×10^4	2.82×10^4	0.770	0.770

Table C2. Stream results of ethyl lactate production of Scenario 2

Parameters	Units	Stream no.						
		1	2	3	4	5	6	7
Temperature	°C	35.0	35.0	35.0	35.0	85.0	79.5	114
Pressure	bar	1.00	1.34	1.00	1.00	1.14	1.00	1.14
Molar Vapor Fraction		0.00	0.00	0.00	0.00	1.00	0.00	0.00
Mole Flows	kmol/hr	477	477	78.1	529	529	907	98.9
Mass Flows	kg/hr	1.43×10^4	1.43×10^4	3.57×10^3	2.43×10^4	2.43×10^4	2.89×10^4	9.71×10^3
Ethanol	kg/hr	0.00	0.00	3.55×10^3	2.42×10^4	2.42×10^4	2.06×10^4	1.18×10^3
Water	kg/hr	7.22×10^3	7.22×10^3	17.8	57.0	57.0	8.29×10^3	6.04
L_1	kg/hr	6.63×10^3	6.63×10^3	0.00	0.00	0.00	19.1	1.21×10^3
L_1E	kg/hr	0.00	0.00	0.00	6.25	6.25	0.01	6.25×10^3
L_2	kg/hr	473	473	0.00	0.00	0.00	0.170	1.02×10^3
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	29.8
Ethylene glycol	kg/hr	0.00	0.00	0.00	1.16	1.16	0.00	1.16

Table C2. Stream results of ethyl lactate production of Scenario 2 (Cont'd)

Parameters	Units	Stream no.						
		8	9	10	11	12	13	14
Temperature	°C	78.0	174	154	35.0	235	80	78.0
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	26.1	72.8	52.8	52.8	20	907	540
Mass Flows	kg/hr	1.20×10^3	8.51×10^3	6.24×10^3	6.24×10^3	2.27×10^3	2.89×10^4	2.16×10^4
Ethanol	kg/hr	1.18×10^3	0.13	0.13	0.13	0.00	2.06×10^4	1.96×10^4
Water	kg/hr	6.03	0.01	0.01	0.01	0.00	8.29×10^3	2.07×10^3
L_1	kg/hr	0.00	1.21×10^3	1.21	1.21	1.21×10^3	19.10	0.00
L_1E	kg/hr	6.25	6.24×10^3	6.24×10^3	6.24×10^3	6.25	0.01	0.00
L_2	kg/hr	0.00	1.02×10^3	0.00	0.00	1.02×10^3	0.17	0.00
L_2E	kg/hr	0.00	29.8	0.00	0.00	29.8	0.00	0.00
Ethylene glycol	kg/hr	0.00	1.16	0.03	0.03	1.13	0.00	0.00

Table C2. Stream results of ethyl lactate production of Scenario 2 (Cont'd)

Parameters	Units	Stream no.						
		15	16	17	18	19	20	21
Temperature	°C	96.6	78.0	35.0	35.0	78.0	157	97.0
Pressure	bar	1.34	1.34	1.34	1.34	1.00	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	368	540	5.39	536	425	651	120
Mass Flows	kg/hr	7.27×10^3	2.16×10^4	334	3.32×10^4	1.95×10^4	3.54×10^4	2.45×10^3
Ethanol	kg/hr	1.02×10^3	1.96×10^4	0.00	0.00	1.95×10^4	78.3	78.3
Water	kg/hr	6.22×10^3	2.07×10^3	0.330	20.9	33.2	2.06×10^3	2.04×10^3
L_1	kg/hr	19.1	0.00	0.00	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.0100	0.00	0.00	0.00	0.00	0.00	0.00
L_2	kg/hr	0.170	0.00	0.00	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.00	333	3.32×10^4	1.16	3.32×10^4	332

Table C2. Stream results of ethyl lactate production of Scenario 2 (Cont'd)

Parameters	Units	Stream no.					
		22	23	24	25	26	27
Temperature	°C	206	35.0	78.0	35.0	78.0	114
Pressure	bar	1.34	1.34	1.00	1.00	1.00	1.34
Molar Vapor Fraction		0.00	0.00	0.00	0.00	1.00	0.00
Mole Flows	kmol/hr	531	531	451	451	529	99.0
Mass Flows	kg/hr	3.29×10^4	3.29×10^4	2.07×10^4	2.07×10^4	2.43×10^4	9.71×10^3
Ethanol	kg/hr	0.00	0.00	2.07×10^4	2.07×10^4	2.42×10^4	1.18×10^3
Water	kg/hr	20.6	20.6	39.2	39.2	57.0	6.04
L_1	kg/hr	0.00	0.00	0.00	0.00	0.00	1.21×10^3
L_1E	kg/hr	0.00	0.00	6.25	6.25	6.25	6.25×10^3
L_2	kg/hr	0.00	0.00	0.00	0.00	0.00	1.02×10^3
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	29.8
Ethylene glycol	kg/hr	3.29×10^4	3.29×10^4	1.16	1.16	1.16	1.16

Table C3. Stream results of ethyl lactate production of Scenario 3

Parameter	Units	Stream no.						
		1	2	3	4	5	6	7
Temperature	°C	35.0	35.0	35.0	35.0	35.0	79.5	166
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.00	1.34
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	122	122	60.1	171	171	231	61.6
Mass Flows	kg/hr	6.82×10^3	6.82×10^3	2.75×10^3	7.84×10^3	7.84×10^3	7.43×10^3	7.22×10^3
Ethanol	kg/hr	0.00	0.00	2.73×10^3	7.81×10^3	7.81×10^3	5.34×10^3	18.0
Water	kg/hr	1.19×10^3	1.19×10^3	13.7	22.2	22.2	2.07×10^3	0.170
L_1	kg/hr	4.24×10^3	4.24×10^3	0.00	0.00	0.00	17.2	496
L_1E	kg/hr	0.00	0.00	0.00	6.25	6.25	0.0800	6.25×10^3
L_2	kg/hr	1.38×10^3	1.38×10^3	0.00	0.00	0.00	0.640	417
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	38.7
Ethylene glycol	kg/hr	0.00	0.00	0.00	0.260	0.260	0.00	0.260

Table C3. Stream results of ethyl lactate production of Scenario 3 (Cont'd)

Parameter	Units	Stream no.						
		8	9	10	11	12	13	14
Temperature	°C	80.8	169	154	35.0	234	79.5	78.0
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	0.450	61.2	52.8	52.8	8.34	231	139
Mass Flows	kg/hr	24.4	7.20×10^3	6.24×10^3	6.24×10^3	958	7.43×10^3	5.60×10^3
Ethanol	kg/hr	17.99	0.00	0.00	0.00	0.00	5.34×10^3	5.08×10^3
Water	kg/hr	0.170	0.00	0.00	0.00	0.00	2.07×10^3	517
L_1	kg/hr	0.00	496	0.500	0.500	496	17.2	0.00
L_1E	kg/hr	6.25	6.24×10^3	6.24×10^3	6.24×10^3	6.25	0.0800	0.00
L_2	kg/hr	0.00	417	0.00	0.00	417	0.64	0.00
L_2E	kg/hr	0.00	38.7	0.00	0.00	38.7	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.26	0.01	0.01	0.24	0.00	0.00

Table C3. Stream results of ethyl lactate production of Scenario 3 (Cont'd)

Parameter	Units	Stream no.						
		15	16	17	18	19	20	21
Temperature	°C	96.5	78.0	35.0	35.0	78.0	158	96.8
Pressure	bar	1.34	1.34	1.34	1.34	1.00	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	92.1	139	1.38	137	110	166	30.0
Mass Flows	kg/hr	1.84×10^3	5.60×10^3	85.3	8.50×10^3	5.07×10^3	9.03×10^3	614
Ethanol	kg/hr	267	5.08×10^3	0.00	0.00	5.06×10^3	20.3	20.3
Water	kg/hr	1.55×10^3	517	0.09	5.22	8.27	514	509
L_1	kg/hr	17.2	0.00	0.00	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.0800	0.00	0.00	0.00	0.00	0.00	0.00
L_2	kg/hr	0.640	0.00	0.00	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.00	85.2	8.49×10^3	0.260	8.49×10^3	84.9

Table C3. Stream results of ethyl lactate production of Scenario 3 (Cont'd)

Parameter	Units	Stream no.			
		22	23	24	25
Temperature	°C	206	35.0	78.0	35.0
Pressure	bar	1.34	1.34	1.00	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	136	136	111	111
Mass Flows	kg/hr	8.41×10^3	8.41×10^3	5.09×10^3	5.09×10^3
Ethanol	kg/hr	0.00	0.00	5.08×10^3	5.08×10^3
Water	kg/hr	5.14	5.14	8.44	8.44
L_1	kg/hr	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.00	0.00	6.25	6.25
L_2	kg/hr	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	8.41×10^3	8.41×10^3	0.260	0.260

Table C4. Stream results of ethyl lactate production of Scenario 4

Parameters	Units	Stream no.						
		1	2	3	4	5	6	7
Temperature	°C	35.0	35.0	35.0	35.0	85.0	79.3	172
Pressure	bar	1.00	1.34	1.00	1.00	1.14	1.00	1.14
Molar Vapor Fraction		0.00	0.00	0.00	0.00	1.00	0.00	0.00
Mole Flows	kmol/hr	141	141	61.4	199	199	271	68.4
Mass Flows	kg/hr	7.89×10^3	7.89×10^3	2.80×10^3	9.12×10^3	9.12×10^3	8.96×10^3	8.06×10^3
Ethanol	kg/hr	0.00	0.00	2.79×10^3	9.09×10^3	9.09×10^3	6.66×10^3	3.74
Water	kg/hr	1.38×10^3	1.38×10^3	14.0	23.2	23.2	2.28×10^3	0.0500
L_1	kg/hr	4.91 v	4.91×10^3	0.00	0.00	0.00	19.1	900
L_1E	kg/hr	0.00	0.00	0.00	6.22	6.22	0.0500	6.22×10^3
L_2	kg/hr	1.60×10^3	1.60×10^3	0.00	0.00	0.00	0.70	894
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	44.7
Ethylene glycol	kg/hr	0.00	0.00	0.00	0.270	0.270	0.00	0.270

Table C4. Stream results of ethyl lactate production of Scenario 4 (Cont'd)

Parameters	Units	Stream no.						
		8	9	10	11	12	13	14
Temperature	°C	89.0	173	154	35.0	236	79.3	78.0
Pressure	bar	1.00	1.34	1.00	1.00	1.34	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	0.140	68.3	52.	52.52	15.8	271	169
Mass Flows	kg/hr	10.00	8.05×10^3	6.20×10^3	6.20×10^3	1.84×10^3	8.96×10^3	6.89×10^3
Ethanol	kg/hr	3.74	0.00	0.00	0.00	0.00	6.66×10^3	6.32×10^3
Water	kg/hr	0.05	0.00	0.00	0.00	0.00	2.28×10^3	570
L_1	kg/hr	0.00	900	0.90	0.90	899	19.1	0.00
L_1E	kg/hr	6.22	6.21×10^3	6.20×10^3	6.20×10^3	6.21	0.0500	0.00
L_2	kg/hr	0.00	894	0.00	0.00	894	0.700	0.00
L_2E	kg/hr	0.00	44.7	0.00	0.00	44.7	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.270	0.0100	0.0100	0.260	0.00	0.00

Table C4. Stream results of ethyl lactate production of Scenario 4 (Cont'd)

Parameters	Units	Stream no.						
		15	16	17	18	19	20	21
Temperature	°C	95.8	78.0	35.0	35.0	78.0	160	96.5
Pressure	bar	1.34	1.34	1.34	1.34	1.00	1.34	1.00
Molar Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flows	kmol/hr	102	169	1.67	166	137	198	33.4
Mass Flows	kg/hr	2.06×10^3	6.89×10^3	103	1.03×10^4	6.31×10^3	1.09×10^4	689
Ethanol	kg/hr	333	6.32×10^3	0.00	0.00	6.30×10^3	25.3	25.3
Water	kg/hr	1.71×10^3	570	0.10	5.77	9.13	567	561
L_1	kg/hr	19.1	0.00	0.00	0.00	0.00	0.00	0.00
L_1E	kg/hr	0.05	0.00	0.00	0.00	0.00	0.00	0.00
L_2	kg/hr	0.70	0.00	0.00	0.00	0.00	0.00	0.00
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene glycol	kg/hr	0.00	0.00	103	1.03×10^4	0.270	1.03×10^4	103

Table C4. Stream results of ethyl lactate production of Scenario 4 (Cont'd)

Parameters	Units	Stream no.					
		22	23	24	25	26	27
Temperature	°C	206	35.0	78.0	35.0	78.1	172
Pressure	bar	1.34	1.34	1.00	1.00	1.00	1.34
Molar Vapor Fraction		0.00	0.00	0.00	0.00	1.00	0.00
Mole Flows	kmol/hr	164	164	137	137	199	68.4
Mass Flows	kg/hr	1.02×10^4	1.02×10^4	6.32×10^3	6.32×10^3	9.12×10^3	8.06×10^3
Ethanol	kg/hr	0.00	0.00	6.30×10^3	6.30×10^3	9.09×10^3	3.74
Water	kg/hr	5.67	5.67	9.17	9.17	23.2	0.0500
L_1	kg/hr	0.00	0.00	0.00	0.00	0.00	900
L_1E	kg/hr	0.00	0.00	6.22	6.22	6.22	6.22×10^3
L_2	kg/hr	0.00	0.00	0.00	0.00	0.00	894
L_2E	kg/hr	0.00	0.00	0.00	0.00	0.00	44.7
Ethylene glycol	kg/hr	1.02×10^4	1.02×10^4	0.270	0.270	0.270	0.270

APPENDIX C UTILITIES SPECIFICATIONS

Table D1. Utilities specifications of ethyl lactate production of Scenario 1, 2, and 3

Utility	Code	Type	Temperature (°C)	
			Inlet	Outlet
Cooling water	CW	Water	20	25
Chilled water	CHILLED	Water	5	10
Low pressure steam	LPS	Steam	125	124
Medium pressure steam	MPS	Steam	175	174
High pressure steam	HPS	Steam	250	249

APPENDIX D EQUIPMENT SPECIFICATIONS

D.1 Heat exchanger specifications

Table D1. Heat exchanger specifications

Scenario	Unit code	Utility type	Utility usage	Heat duty	Area
			(kg/hr)	(kW)	(m^2)
1	E-101	CW	7.14×10^4	414	27.6
	E-102	CW	6.55×10^5	3.80×10^3	201
	E-103	CW	1.36×10^5	791	92.6
2	E-101	CW	7.15×10^4	415	27.6
	E-102	CW	7.66×10^5	4.44×10^3	235
	E-103	CW	1.25×10^5	726	85.0
	E-104	LPS	1.09×10^4	6.61×10^3	70.8
3	E-101	CW	7.15×10^4	4.5	27.6
	E-102	CW	1.96E+05	1.14×10^3	60.0
	E-103	CW	3.08×10^4	178	20.9
4	E-101	CW	7.11×10^4	412	27.4
	E-102	CW	2.37×10^5	1.37×10^3	72.6
	E-103	CW	3.82×10^4	221	29.6
	E-104	LPS	4.08×10^3	2.49×10^3	26.6

D.2 Distillation column specifications

Table D2. Heat exchanger of distillation column specifications

Scenario	Unit code	Unit name	Utility type	Utility usage (kg/hr)	Heat duty (kW)
1	T-101	Condenser	CW	1.70×10^{6}	-9.86×10^{3}
		Reboiler	LPS	2.00×10^{4}	1.22×10^{4}
	T-102	Condenser	CW	3.07×10^{5}	-1.78×10^{3}
		Reboiler	HPS	4.49×10^{3}	2.14×10^{3}
	T-103	Condenser	CW	1.48×10^{5}	-859
		Reboiler	HPS	1.85×10^{3}	884
	T-104	Condenser	CW	1.45×10^{6}	-8.39×10^{3}
		Reboiler	LPS	1.40×10^{4}	8.54×10^{3}
	T-105	Condenser	CW	7.42×10^{5}	-4.30×10^{3}
		Reboiler	MPS	1.24×10^{4}	7.00×10^{3}
	T-106	Condenser	CW	3.16×10^{5}	-1.83×10^{3}
		Reboiler	HPS	6.23×10^{3}	2.98×10^{3}
2	T-101	Condenser	CW	1.79×10^{6}	-1.04×10^{4}
		Reboiler	LPS	9.79×10^{3}	5.96×10^{3}
	T-102	Condenser	CW	6.50×10^{4}	-377
		Reboiler	HPS	1.41×10^{3}	673
	T-103	Condenser	CW	1.44×10^{5}	-835
		Reboiler	HPS	1.79×10^{3}	856
	T-104	Condenser	CW	2.03×10^{6}	-1.18×10^{4}
		Reboiler	LPS	1.96×10^{4}	1.19×10^{4}
	T-105	Condenser	CW	8.95×10^{5}	-5.19×10^{3}
		Reboiler	MPS	1.49×10^{4}	8.44×10^{3}
	T-106	Condenser	CW	3.19×10^{5}	-1.85×10^{3}
		Reboiler	HPS	6.45×10^{3}	3.08×10^{3}

Scenario	Unit code	Unit name	Utility type	Utility usage (kg/hr)	Heat duty (kW)
3	T-101	Condenser	CW	4.61×10^5	-2.67×10^3
		Reboiler	HPS	8.66×10^3	4.14×10^3
	T-102	Condenser	CW	3.23×10^4	-187
		Reboiler	HPS	414	198
	T-103	Condenser	CW	1.39×10^5	-806
		Reboiler	HPS	1.66×10^3	793
	T-104	Condenser	CW	5.43×10^5	-3.15×10^3
		Reboiler	LPS	5.23×10^3	3.18×10^3
	T-105	Condenser	CW	2.33×10^5	-1.35×10^3
		Reboiler	MPS	3.87×10^3	2.19×10^3
	T-106	Condenser	CW	8.02×10^4	-465
		Reboiler	HPS	1.63×10^3	777
4	T-101	Condenser	CW	5.40×10^5	-3.13×10^3
		Reboiler	HPS	9.19×10^3	4.39×10^3
	T-102	Condenser	CW	3.57×10^4	-207
		Reboiler	HPS	439	209
	T-103	Condenser	CW	1.41×10^5	-818
		Reboiler	HPS	1.74×10^3	830
	T-104	Condenser	CW	7.51×10^5	-4.35×10^3
		Reboiler	LPS	7.21×10^3	4.39×10^3
	T-105	Condenser	CW	2.92×10^5	-1.69×10^3
		Reboiler	MPS	4.81×10^3	2.72×10^3
	T-106	Condenser	CW	9.15×10^4	-530
		Reboiler	HPS	1.87×10^3	895

D.3 Reactive distillation column configuration

Table D3. Configuration of the reactive distillation column, T-101.

Property	Unit	Scenario 1			Scenario 2		
		Rectifying	Reactive	Stripping	Rectifying	Reactive	Stripping
Section starting stage	-	2	7	36	2	7	36
Section ending stage	-	6	35	39	6	35	39
Internal type	-	Trayed	Packed	Trayed	Trayed	Packed	Trayed
Tray/Packing type	-	Sieve	Mellapak	Sieve	Sieve	Mellapak	Sieve
Tray spacing	m	0.610	-	0.610	0.610	-	0.610
HETP	m	-	0.600	-	-	0.600	-
Section diameter	m	2.08	1.86	2.47	2.24	1.76	1.71
Section height	m	3.05	17.4	2.44	3.05	17.4	2.44

Property	Unit	Scenario 3			Scenario 4		
		Rectifying	Reactive	Stripping	Rectifying	Reactive	Stripping
Section starting stage	-	2	7	36	2	7	36
Section ending stage	-	6	35	39	6	35	39
Internal type	-	Trayed	Packed	Trayed	Trayed	Packed	Trayed
Tray/Packing type	-	Sieve	Mellapak	Sieve	Sieve	Mellapak	Sieve
Tray spacing	m	0.610	-	0.610	0.610	-	0.610
HETP	m	-	0.600	-	-	0.600	-
Section diameter	m	1.09	1.04	1.35	1.19	1.07	1.43
Section height	m	3.05	17.4	2.44	3.05	17.4	2.44

APPENDIX E ECONOMIC ANALYSIS RESULTS

Table E1. Economic analysis parameters

Name	Units	Value
Number of weeks per period	Weeks/year	52
Number of periods for analysis	-	20
Tax rate	%/year	20
Interest rate	%/year	20
Economic life of project	year	20
Salvage value	%	20
Project capital escalation	%/year	5
Products escalation	%/year	5
Operating and maintenance labor escalation	%/year	3.5
Utilities escalation	%/year	3
Material indexing	-	1.14
Length of start-up period	Weeks	20
Operating hours per period	Hours/year	8,000

Table E2. Economic results

Items	Units	Scenario			
		1	2	3	4
Total capital cost	USD	2.26×10^7	2.72×10^7	1.60×10^7	1.85×10^7
Total operating cost	USD/y	1.72×10^8	1.68×10^8	1.37×10^8	1.58×10^8
Total raw materials cost	USD/y	1.43×10^8	1.38×10^8	1.20×10^8	1.37×10^8
Total utilities cost	USD/y	1.46×10^7	1.61×10^7	5.36×10^6	7.36×10^6
Total product sales	USD/y	1.74×10^8	1.74×10^8	1.74×10^8	1.74×10^8
Net present value	USD	7.82×10^6	2.48×10^7	1.76×10^8	7.72×10^7
Internal rate of return	%	21.3	24.1	74.6	37.9
Payout period	y	17.2	13.2	3.41	6.79

VITA

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