The Hilltop Review

Volume 9
Issue 2 *Spring*

Article 12

June 2017

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Preferred Citation Style (e.g. APA, MLA, Chicago, etc.)
APA

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Cover Page Footnote

I would like to offer my thanks to Dr. Kline for his support and advice during the process of this research. I would also like to thank Western Michigan University, Chemical Engineering program. I would like to thank my family for their support during this research . And finally, I would like to thank Jessica Postma for her review of this research.

Acetone Production

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Introduction

THE intention of establishing an acetone factory particularly within the city of Basra, Iraq, is meant to satisfy three specific purposes. First, Iraq is geographically located between Europe, the Arabian Gulf, and west Asia; therefore, it is centrally situated and thus presents an opportune location for exporting acetone. Second, Iraq's budget is entirely dependent on the production of petroleum. However, numerous factories have struggled with production costs and a lack of government funding due to various wars, terrorist activities, and globally fluctuating oil prices. In addition, and most notably, petroleum is a limited natural resource (Moore & Parker, 2007). The foremost question the Iraqi government faces is how best to manage this issue. Arguably, the acetone production factory suggested in this study can satisfy the country's economic needs and increase Iraq's budget since it would be a profitable project. Third, one of the largest cities in Iraq, Basra, has been chosen for the production factory location due to its close proximity to countries where raw materials can be acquired. In addition, the proposed factory location is near the Euphrates, Tigris, and Arabian Gulf. These bodies of water can be used as a source for the cooling and heatingsystems.

Table 1: Consumption of Acetone (2005) (PubChem)

Acetone Consumption (Global Demand)	5 Million Tons per Year
As a solvent	31%
Acetone cyanohydrin (MMA)	30%
Bisphenol A	20%
Aldol chemicals	11%
Other uses	8%

The factory is designed theoretically with a low cost based on the calculations presented in the Results section. Moreover, the raw material is isopropyl alcohol and water. The reaction is endothermic. Therefore, the reaction needs a certain amount of heat to decompose the H-atom from the isopropyl alcohol.

Acetone is a colorless liquid that is a very important solvent for some kinds of fibers and plastics. Acetone is one of the most vital materials due to its many different uses and purposes. The main use for acetone is in the production of methyl methacrylate and bisphenol A (BPA (. Acetone is also used as a solvent in the pharmaceutical industry and in the production of synthetic fibers, in the preparation of metal before painting, in the application of biological research, and in the cleaning of various materials and surfaces, including cleaning residue from glass, laboratory tools, fibers, and as nail polish remover (Hudson, 2015; Coulson et al., 1999b).

However, acetone is toxic and flammable, so it should be kept away from any source of fire or ignition due to its flammable chemical nature. It should be stored in a safe environment, and pregnant women and children should avoid working with it. In addition, those who work with acetone gas should be careful since acetone can dry out skin and cause other health issues like eye sensitivity.

Methodology

There are many methods to synthesize acetone. One of the most efficient methods is the decomposition of isopropyl alcohol, which is the proposed method in this project. Another method to synthesize acetone is called the cumene process, in which benzene (C6H6) reacts with propylene (C3H6) to form cumene (C9H12). After reaction, cumene is oxidized to form acetone (CH3)2CO with phenol (C6H6O), as is clarified in the equations below (Hudson, 2015; Coulson et al., 1999b). The cumene process method is quite expensive, since it requires the raw materials and extra separation equipment to separate acetone from many different materials (Moore & Parker, 2007; Coulson et al., 1999b). Therefore, this study focuses on the more economic method of decomposition of isopropyl alcohol over the cumene process method.

$$C_6H_6 + C_3H_6 \rightarrow C_9H_{12}$$

$$C_9H_{12} + O_2 \rightarrow (CH_3)_2CO + C_6H_6O$$

The proposed method in this project is the decomposition of isopropyl alcohol (C3H8O) with water (H2O) as a catalyst—water is not reacted with isopropyl alcohol. Isopropyl alcohol (C3H8O) and water (H2O) together enter the reaction at 298 K (25°C) with 101.325 kPa (1 bar). In these conditions, the reaction is endothermic. The heat is supplied to the Plug Flow Reactor (PFR) via hot water at 700 K, with hot water supplied from a fired heater. The produced materials from the reaction are acetone (C3H6O) and hydrogen (H2), and the amount of acetone produced at 63346 kmol/hr (Table 4) (Coulson et al., 1999b; Scorecard).

$$C_3H_8O \xleftrightarrow{H_2O} C_3H_6O + H_2$$

Design Process

In designing a factory, the most crucial component is choosing the method to use in production. Following that, the tools and equipment required for the factory must be selected based on the physical properties of the consumed and produced materials. After that, calculations should be done before establishing the factory, including technical and economic feasibility. The acetone factory requires the following equipment, for the proposed process that is shown in Appendix A.

Equipment

Reactor (R)

The Plug Flow Reactor (PFR) is the most suitable reactor for the following reasons: PFR is used for large scale, fast reactions; continuous production; high temperatures; high conversion per unit volume; low operating labor (cost); and efficient heat transfer. The feed enters into the reactor at 298 K, the operation pressure of the reactor is 800 kPa (8 bar), and the operation temperature of the reactor is 499 K (225.85°C). The reactor has 53 tubes (Levenspiel, 1999).

The reaction

The reaction is endothermic. Ninety percent of isopropyl alcohol converts to acetone and hydrogen after decomposition of the H - atom from isopropyl alcohol. The reaction takes place in the tubes, with a significant amount of heat added to the reactor by hot water. The source of heat is from the fired heater, which operates at 700 K and 800 kPa (8 bar). In addition, the heat transfers from outside the tubes to inside the tubes by conduction. The outlet pipe from the reactor (Stream 4) goes to the heat exchanger (HE-1) (Appendix A) (Levenspiel, 1999).

Heat Exchanger 1 (HE-1)

The function of the HE-1 is to cool Stream 4, since Stream 4 comes out of the reactor with a high temperature of 450 K. The temperature needs to be reduced because the next unit after the reactor is the distillation column. In the distillation column, hydrogen (H_2) is the first component that leaves the mixture, because H_2 has the lowest boiling point. In addition, if Stream 4 enters the distillation column at 450 K, all components will be evaporated. This would be unproductive since the function of distillation separates the components based on the difference in boiling points. Therefore, Stream 4 must enter the heat exchanger (HE-1) at 450 K and leave HE-1 at 278 K,which is the temperature of Stream 5. Water is used to cool the mixture in HE-1 (Richardson et al., 2002).

Distillation Column 1 (D-1)

Reactors are usually followed by a separation unit. In this process, a distillation column is proposed to separate the components due the materials' very different boiling points. Stream 5 enters the distillation column as a liquid mixture with a temperature of 278 K. In this distillation column, the temperature of the mixture is greater than the boiling point of hydrogen, which results in the hydrogen's evaporation. When the temperature of the distillation reaches the boiling points of H_2, the H_2 transfers to the upper part of distillation and then is condensed (Richardson et al., 2002).

Condenser 1 (C-1)

H_2 along with a small amount of acetone, isopropyl alcohol, and water release to the top of the distillation in a vapor phase. The condenser liquidizes the materials to return to the distillation in a liquid phase. The condenser cools the vapor mixture as reflux materials. However, five percent of acetone remains in a gas phase with H_2. Five percent of acetone accompanies H_2 out of the condenser to the refrigeration unit (R-1) (Richardson et al., 2002).

Boiler 1 (B-1)

In the first distillation, the operation temperature should be greater than the boiling point of H_2. A boiler is required to warm the mixture. The boiler evaporates the amount of H_2 that is not evaporated through the first step of distillation since the system is continuous (Richardson et al., 2002; Sinnott, 2005a).

Refrigeration Unit 1 (R-1)

The output of the first condenser (C-1) is a mixture of H_2 and five percent of acetone. The mixture must be liquidized in order to separate the small amount of acetone. Refrigeration cools the H_2 into a liquid phase to efficiently store it, and then the acetone is liquidized and separated into Stream 7. Furthermore, acetone is re-mixed with the components from the boiler (B-1) in Stream 9 (Appendix A) (Richardson et al., 2002).

Heat Exchanger 2 (HE-2)

A shell and tube heat exchanger is used to heat Stream 10. Stream 10 has to be warmed to reach the boiling point of the material that should be separated, from 274 K to 347 K. Heating Stream 10 is done by using hot water through HE-2. The outlet from HE-2 is Stream 11, which enters the second distillation column (Appendix A) (Richardson et al., 2002; Sinnott, 2005a).

Distillation Column 2 (D-2)

Stream 11 enters the second distillation column at 347 K. The operation temperature of the distillation column reaches the boiling point of acetone, at 329.2 K (56.2°C). Acetone is evaporated with a small amount of isopropyl alcohol, and a small portion of isopropyl alcohol is separated from the acetone and raised to the top of the distillation. In turn, isopropyl alcohol returns to the distillation as reflux material through the condenser (C-2). Water and isopropyl alcohol leave the column from the bottom. This distillation column also has a boiler at the bottom and a condenser at the top (Richardson et al., 2002).

Condenser 2 (C-2)

The condenser cools the vapor mixture of acetone and isopropyl alcohol. In addition, the amount of isopropyl alcohol returns to the distillation as reflux material. Then acetone is produced in Stream 14 (Appendix A). The purpose of using the second refrigerator is to turn acetone from a gas phase to a liquid phase due to the difficulty of storing acetone as a gas. The amount of the produced acetone from C-2 is 63346 kmol/hr, which is stored in Vessel 2, as shown in Table 4 (Richardson et al., 2002).

Boiler 2 (B-2)

The function of the boiler is to heat the rest of the acetone to reach its boiling point. Acetone then separates from the mixture. The operation temperature of the second distillation column is established based on the boiler (Richardson et al., 2002).

Heat Exchanger 3 (HE-3)

To reach the boiling point of isopropyl alcohol, Stream 16 is heated before the mixture enters the third distillation column by HE-3. The process principle is the same as the previous heat exchangers as well as the same design. All of the exchangers are called shell and tube heat exchangers, a kind of heat exchanger that is distinguished by the high efficiency of heat transfer because the amount of heat distributes over the number of tubes, which makes the heat transfer occur more quickly (Sinnott, 2005a).

Distillation Column 3 (D-3)

Isopropyl alcohol is separated from water through D-3 after the operation temperature reaches the boiling point of isopropyl alcohol. Isopropyl alcohol transfers up to D-3 with a small amount of water. In tandem, the water transfers down D-3 with a small amount of isopropyl alcohol (Richardson et al., 2002).

Condenser 3 (C-3)

The vapor mixture is cooled, and isopropyl alcohol is separated from the rest of the water. Isopropyl alcohol leaves C-3 in a vapor phase to a refrigeration unit (R-3), and water returns to D-3 and then leaves the distillation column through Stream 19 (Richardson et al., 2002).

Boiler 3 (B-3)

The boiler's function is to warm the mixture and to maintain the operation temperature of D-3 in order to reach the boiling point of isopropyl alcohol. This boiler warms the mixture at the boiling point of isopropyl alcohol, and then isopropyl alcohol evaporates and transfers to the top of the distillation column. The refrigerator then turns the isopropyl alcohol from a vapor phase to a liquid phase and it is recycled to the reactor (Richardson et al., 2002).

Waste Stream

There are three components of the waste stream in this process. First, the hydrogen (Stream 8) is separated from the first distillation column; hydrogen can be a byproduct. All the focus in this study is on acetone production, therefore the technical and economic feasibility of hydrogen is not studied. Second, isopropyl alcohol is separated from the third distillation column; because this component feeds the reactor, it is recycled from the third distillation column to the reactor through Stream 21 (Figure 1). Finally, the water component is separated from the third distillation column, which could be used as catalyst for the reactor. However, water is not recycled to the reactor in this process for two reasons. The distance between the third distillation column and the reactor is quite far, as demonstrated in Table 2. To recycle water from the third distillation column to the reactor could be quite expensive, given the need to provide and install the pipe with valves, as well as provide for periodic maintenance (Richardson et al., 2002).

Table 2: Anticipated Minimum Space between the Equipment

Equipment	Equipment	Space (m)
Reactor	Heat Exchanger 1	12
Reactor	Fired heater	12
Heat Exchanger 1	Distillation 1	3
Distillation 1	Refrigerator 1	3
Distillation 1	Heat Exchanger 2	3
Heat Exchanger 2	Distillation 2	3
Distillation 2	Refrigerator 2	3
Distillation 2	Heat Exchanger 3	3
Heat Exchanger 3	Distillation 3	3
Distillation 3	Refrigerator 3	3
Refrigerator 3	Vessel 1	6
Vessel 1	Pump 1	3
Reactor	Ancillary Buildings	100
Refrigerator 2	Vessel 2	6

Table 3: Boiling Points

Component	BP (K°)	BP (C°)
2-propanol	355.2	82.2
H_2O	373	100
Acetone	329.2	56.2
H_2	20.2	-252.8

Results and Discussion

The mole flow rate is calculated for each material in each stream, as shown in Table 4. The amount of heat for each piece of equipment is shown in Table 5. Pressure and temperature are calculated for each piece of equipment and stream. Antonio equations and constants are used to calculate the pressures and temperatures (Richardson et al., 2002; Sinnott, 2005b).

$$\text{2-Propanol} \xleftrightarrow[\text{B}]{\text{H}_2\text{O}} \text{Acetone} + \text{Hydrogen}$$

$$\text{A} \longleftrightarrow \text{C} + \text{D}$$

Let A = 2-propanol, B = Water, C = Acetone, and D = Hydrogen

After calculating the total mole flow rate for each stream, the change in enthalpy can be calculated by using Antonia equations with Raoult's Law.

Antonia equations:

$$\Delta H = n \int_{T_{ref}}^{T_i} Cp\,dT \quad (1)$$

$$CP = A + BT + CT^2 + DT^3 \quad (2)$$

$$\log(P_i^*) = A - \frac{B}{CT_i} \quad (3)$$

Raoult's Law:

$$P_i^* = P_T * Y_i \quad (4)$$

Y_i = mole of (i) / total no. of moles (5)

The amount of heat for each piece of equipment is calculated through Equation 6, and the added heat amount of the reactor is calculated through Equation 7:

For equipment: $Q = \sum \Delta H\ in - \sum \Delta H\ out \quad (6)$

For the reactor: $\sum \Delta H_{in(Reactor)} + Q = \Delta Hr + \sum \Delta H_{out(Reactor)} \quad (7)$

Table 4: Material and Energy Balance Results

Stream	Component (kmol/hr)				Pressure	Temp
	2-Propanol	H2O	Acetone	H_2	kPa	K
1	63033.74	32164.85	-----------	-------------	101.325	288
2	62500	32164.85	----------	-------------	101.325	298
3		15852.7	----------	------------	800	700
4	6944.44	32164.85	62499.99	62499.99	750	450
5	6944.44	32164.85	62499.99	62499.99	400	278
6	------------	---------	3282.184	62499.99	600	60
7	------------	--------	3282.184	------------	300	40
8	------------	----------	---------	62499.99	300	40
9	6944.44	32164.85	60063.9	---------	600	466
10	6944.44	32164.85	63346	---------	205	274
11	6944.44	32164.85	63346	---------	224	347
12	630	----------	63346	----------	224	333.6
13	630	----------	----------	---------	150	310
14	----------	---------	63346	---------	150	310
15	6314.44	32164.85	---------	----------	224	361
16	6944.44	32164.85	----------	-----------	150	280
17	6944.44	32164.85	------------	------------	170	370
18	6944.44	-----------	------------	------------	110	355.4
19	------------	32164.85	------------	------------	140	382.5
20	6944.44	-----------	------------	------------	101.325	310
21	6944.44	-----------	------------	------------	150	320

Table 5: The Amount of Heat (Q) for the Major Pieces

Pieces	Symbol	Q (MJ/hr)
Reactor	R	$3.5783*10^6$
Distillation 1	D-1	847702.059
Distillation 2	D-2	56623.17745
Distillation 3	D-3	5497.0043
Heat Exchanger 1	H.E-1	$3.5828*10^5$
Heat Exchanger 2	H.E-2	800965.6423
Heat Exchanger 3	H.E-3	10319.0527
Refrigerator 1	RF-1	$2.29*10^6$
Refrigerator 2	RF-2	178611.1377
Refrigerator 3	RF-3	6961.601
Pump 1	P-1	56556.10861

Economic Feasibility

The cost of the factory, in U.S. dollars, is shown in detail in Tables 6, 7, and 8. This acetone production factory is profitable since ROI is 1.13, which is greater than one (ROI >1), as shown in Table 7. The production of acetone from this factory is 63346 kmol / hr, which is a significantly high amount, and it meets the needs of acetone demand in Iraq and the Middle Eastern region for export (Index of process equipment; Process equipment costs; ICIS; ReAgent).

Table 6: Expenses in U.S. Dollars per Year

Raw material	354,710,993
Maintenance	1,498,986.711
Supplies	1,316,183.453
Operating labor	2,920,000
Burden	2,211,075.387
Utilities	2,200,000
Supervisory and other labor	438,000
Catalyst	15,000
Auxiliaries	1,241,606.515
Patent and royalty charge	1,096,819.54
Cooperate overhead	1,097,008.169
Ad valoreum tax	1,096,819.544
Research expenses	731,213.02
Total expenses	370,573,705.3

Table 7: Cash Flow Summary

Symbol	Value or scale
TCI	96560651.48
PP	1.161
Average Annual Cash Flow	83116087 $
B/C	11.64
Summation (+DCF)	582237170 $
(B/C) modified	6.03
Summation (+cash flow)	1124928698 $
Average profit	109212804 $
ROI	1.13

Table 8: Purchased Equipment Cost (PEC) in U.S. Dollars

Equipment	Symbol	Cost F.O.B.	Cost for Delivering and Installment
Reactor	R	111700	662,381
1st heat exchanger	HE-1	42000	249,060
2nd heat exchanger	HE-2	37647.88	223,251.9
3rd heat exchanger	HE-3	30394.8	180,241.16
Re-boiler-1	B-1	20000	118,600
Re-boiler-2	B-2	17758.17	105,305.94
Re-boiler-3	B-3	15653.09	92,822.82
1st refrigerator	R-1	79600	472,028
2nd refrigerator	R-2	79600	472,028
3rd refrigerator	R-3	79600	472,028
1st condenser	C-1	37900	224,747
2nd condenser	C-2	32167.7	190,754.46
3rd condenser	C-3	22136.47	131,269.26
1st distillation column	D-1	199040.4	1,180,309.5
2nd distillation column	D-2	176462	1,046,419
3rd distillation column	D-3	124018.8	735,431.4
The fired heater	FH	10000	59,300
The pump	P-1	8400	49,812
1st vessel	V-1	69100	409,763
2nd vessel	V-2	39894.9	236,576.757
Total of PEC		1,233,074.21	7,312,130.296

Conclusion

As stated, the proposed method is the thermal decomposition for isopropyl alcohol (Coulson et al., 1999b). This method is one of the more affordable methods used to produce acetone. In addition, the amount of produced acetone is 63346 kmol/hr, as shown in Table 4. In this method, only this one raw material is needed, and it should be used with water as inert to produce acetone, wherein water does not react but works as a catalyst. In contrast, the cumene process is significantly more expensive, particularly in the provision of raw materials and extra equipment. This is the justification for why this study has focused on the isopropyl alcohol decomposition method rather than the cumene process method.

The factory is proposed to be constructed in Basra City, Iraq, with the Euphrates and Tigris Rivers providing the water for the factory's cooling and heating systems. During the steps of production, hydrogen is formed in the factory. The hydrogen can be considered a second productive material to be utilized in different fields. However, the primary purpose of this factory is acetone production. In addition to the accessibility of raw materials, the other primary reason to establish acetone production in Iraq is economic. The proposed factory is profitable due to the positive long term economic implications in regard to the return on investment (ROI=1.13). The average profit for six years of running the factory is $109,212,804, as demonstrated in Table 7.

Recommendation

As previously discussed, another benefit of this factory is the production of hydrogen. While this factory concept focuses exclusively on the production of acetone, it can also be utilized for the production of hydrogen as it is produced from the first distillation column. Essentially, it can be beneficial to utilize the hydrogen with less cost since it is already produced as a byproduct in this process. This additional concept would need to have designed unit operations to extract and store the hydrogen.

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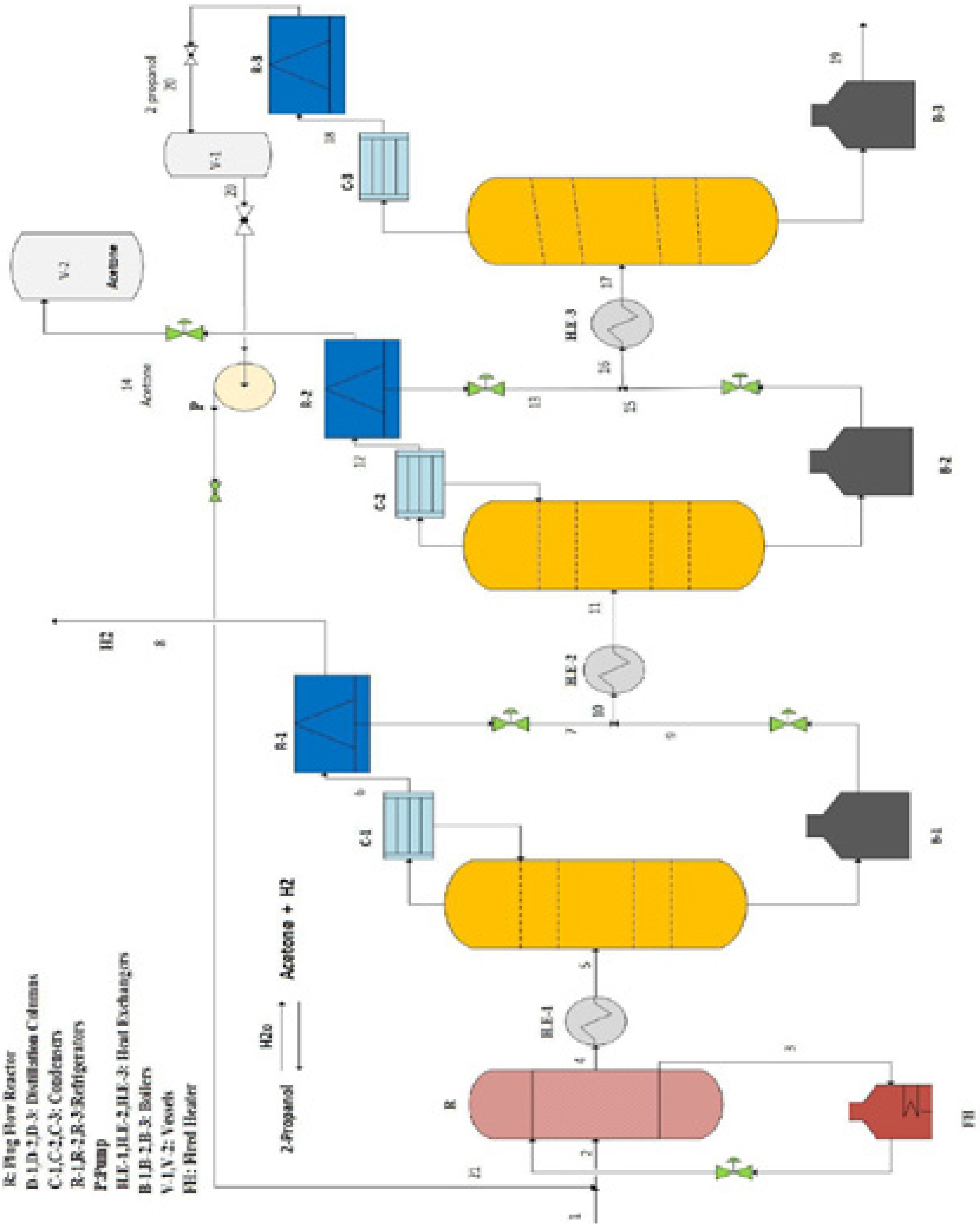
Appendix A

Layout of Acetone Factory



Appendix B

Nomenclature

Q°: Volumetric Flow Rate m3/hr

Q: The Amount of Heat Transfer (KJ/kmol)

EUAC: Equivalent Uniform Annual Cost

PP: Payback Period

TCI: Total Capital Investment

FCI: Fixed Capital Investment

WC: Working Capital

ROI: Return on Investment BFIT

DEP: Depreciation

BV: Book Value

EXP: Expenses

INV: Investment

PEC: Purchased Equipment Cost

NTU: Number of Transfer Units

DF: Discount Factor DCF: Discount Cash Flow

NPV: Net Present Value

CF: Cash Flow

EUAW: Equipment Uniform Annual Worth

ΔHEnthalpy Change

ΔHrThe Enthalpy Change of a Reaction

P_T : Total Pressure

P_i : Vapor Pressure for component i

Y_i : The vapor Mole Fraction of Component i