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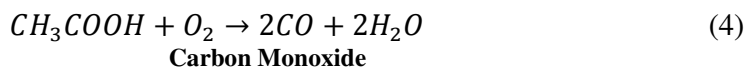
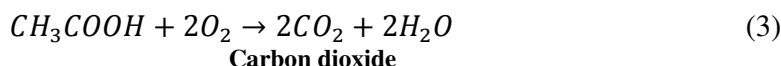
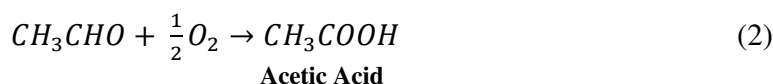
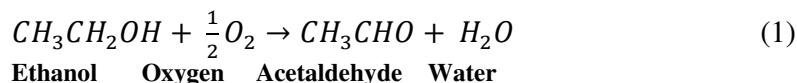
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Introduction

Acetic acid has many different uses in the chemical industry. It is one of the main ingredients in vinegar, and is mainly used as a reagent in further chemical processing, such as the production of cellulose ethanoate and polyester [1]. Acetic Acid is mildly explosive in certain environments and can cause harmful effects if contact with bare skin or mucous membranes occurs, so the production process must be designed carefully and all safety aspects must be taken into consideration.

Production of acetic acid can be done in many ways, the most common being methanol carbonylation. Monsanto was the first to develop the rhodium and iodide catalyst process to expedite the carbonylation process. Developments to this process have been made since it was created, such as the advancement of the Catvia by BP, which uses iridium to produce fewer byproducts [2].

Another way acetic acid can be produced is the dehydrogenation of ethanol, which will be the design discussed in this report. In this method, the ethanol is oxidized to acetaldehyde, which is then further oxidized into acetic acid. This method is arguably the first process created for the production of acetic acid, and continues to be developed in the modern chemical industry. The reaction sequence can be shown below.



The chemical engineering team was tasked with designing a process using the dehydrogenation of ethanol method to produce at least 10,000 kg of acetic acid with a purity of 99.5%. This is to be done using an ethanol recycle system with an input of 10,000 kg with a composition of 99.9% ethanol, and 0.01% water. This stream is fed to a reactor, along with the oxidant stream of air, with tubes of dimensions 0.125 inches in diameter and 6 m long. The expected conversion of ethanol is 80% per pass, and 92% of acetaldehyde per pass. Less than 5% of water is required to be in the final product stream, as well as less than 5 ppm of ethanol and acetaldehyde. The process was also designed to include minimal carbon dioxide and carbon monoxide in the final product. The excess reactants were also expected to have a recovery rate from adsorption at 99.9% for a recycle stream back to the reactor.

Previously constructed designs have been considered for the ethanol method, such as using a drying separation column to purge the product of water and then further separating out the hydrocarbons in a secondary column. Another design considered was separating the residual water and product in a preliminary column, and then further separating the hydrocarbons for recycle to produce more acetic acid. This design further studies the latter method due to the complexity of the ethanol/water separation caused by an azeotrope.

The design process has been simulated by using Aspen Plus software, as well as calculations and heuristics of the equipment. Included in this report is a process flow diagram, detailed cost analysis, rigorous equipment design, utility summary, and the discussion of the design decisions.

Design Conditions

As stated previously, the assignment for the chemical engineering team was to design the production of acetic acid from ethanol dehydrogenation starting with a 10,000 kg liquid ethanol-water stream. The requirement for the product was to produce at least 10,000 kg of acetic acid with a 99.5% purity with less than 0.5% water. The feed conditions given are shown in the table below.

Table 1: Process Feed conditions for the Production of Acetic Acid

Component	Composition	Flow Rate (kg/hr)	Pressure (bar)	Temperature (C)
Ethanol	99.9%	9990	2	25
Water	0.01%	10	2	25

The reactor given for this process is a multi-tube quasi-isothermal fixed-bed reactor with tubes that have dimensions of 6 m long and 25 mm in outer diameter. 80% of the ethanol must be converted per pass, as well as 92% of the acetaldehyde. The reactor inlet must contain 35 mol/mol for air/hydrocarbons in order to reduce the chances of an explosion. The reactor effluent must contain 0.23 mol/mol for CO₂ to acetic acid, and 0.08 mol/mol for CO to acetic acid. Because of the sensitivity of the catalyst, the gas entering the reactor must not fall below 200°C. This is due to water condensing and deactivating the catalyst.

Another specification given to the chemical engineering team was to design a heat exchanger that crosses the reactor effluent and input streams with the initial air/ethanol mixture in order to save on utility costs. From this exchanger, the reactor effluent is cooled and separated. It was given as a requirement that 99.9% of the excess acetaldehyde, water, and ethanol is recovered and recycled back to the system. The specification for the rigorously designed columns was that the average flooding per diameter section must be approximately 70%. This will prevent the design from being in danger of flooding or drying up. These conditions must be met in order for the design to be considered.

Because only certain utilities were available for the plant design, the chemical engineering team used the best three available sources of heating and cooling: low pressure steam, cooling water, and chilled water. The low pressure steam conditions were given as being at 8 bar. The cooling water was available as coming in at 30°C and exiting at 40°C. The chilled water was available as entering at 5°C and exiting at 15°C.

Stream Summary

The following tables show the stream summary results of the Aspen model.

Table 2: Stream summaries for streams 1-5

Stream Number	1	2	3	4	5
Phase	Mixed	Liquid	Liquid	Vapor	Vapor
Temperature (°C)	38	38	38	126	220
Pressure (bar)	2	2	8	8	8
Molar Vapor Fraction	0	0	0	1	1
Mole Flows (kmol/hr)	308	308	308	10511	10511
Component Mole Fractions					
ETHANOL	0.869	0.869	0.869	0.025	0.025
WATER	0.067	0.067	0.067	0.002	0.002
CO2	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000
AA	0.000	0.000	0.000	0.000	0.000
ACETA-01	0.060	0.060	0.060	0.002	0.002
N2	0.003	0.003	0.003	0.768	0.768
O2	0.001	0.001	0.001	0.203	0.203
Mass Flows (kg/hr)	13558	13558	13558	307878	307878
Component Mass Fractions					
ETHANOL	0.910	0.910	0.910	0.040	0.040
WATER	0.027	0.027	0.027	0.001	0.001
CO2	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000
AA	0.000	0.000	0.000	0.000	0.000
ACETA-01	0.060	0.060	0.060	0.003	0.003
N2	1.948E-03	1.948E-03	1.948E-03	7.344E-01	7.344E-01
O2	6.477E-04	6.477E-04	6.477E-04	2.217E-01	2.217E-01

Table 3: Stream summaries for streams 7-12

Stream Number	6	8	9	10	12
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Phase	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature (°C)	176	35	270	175	178
Pressure (bar)	3	3	6	8	6
Molar Vapor Fraction	1	1	1	1	1
Mole Flows (kmol/hr)	10203	10203	10547	10203	10547
Component Mole Fractions					
ETHANOL	0.000	0.000	0.005	0.000	0.005
WATER	0.000	0.000	0.028	0.000	0.028
CO2	0.000	0.000	0.004	0.000	0.004
CO	0.000	0.000	0.001	0.000	0.001
AA	0.000	0.000	0.018	0.000	0.018
ACETA-01	0.000	0.000	0.002	0.000	0.002
N2	0.791	0.791	0.765	0.791	0.765
O2	0.209	0.209	0.177	0.209	0.177
Mass Flows (kg/hr)	294320	294320	307878	294320	307878
Component Mass Fractions					
ETHANOL	0.000	0.000	0.008	0.000	0.008
WATER	0.000	0.000	0.017	0.000	0.017
CO2	0.000	0.000	0.006	0.000	0.006
CO	0.000	0.000	0.001	0.000	0.001
AA	0.000	0.000	0.036	0.000	0.036
ACETA-01	0.000	0.000	0.003	0.000	0.003
N2	0.768	0.768	0.734	0.768	0.734
O2	0.232	0.232	0.194	0.232	0.194

Table 4: Stream summaries for streams 13-17

Stream Number	13	14	15	16	17
Phase	Vapor	Mixed	Liquid	Vapor	Liquid
Temperature (°C)	178	30	40	40	40
Pressure (bar)	4	4	4	4	4
Molar Vapor Fraction	1	1	0	1	0
Mole Flows (kmol/hr)	10547	10547	331	10217	218
Component Mole Fractions					
ETHANOL	0.005	0.005	0.050	0.004	0.168
WATER	0.028	0.028	0.536	0.011	0.521
CO2	0.004	0.004	0.000	0.004	0.000
CO	0.001	0.001	0.000	0.001	0.000
AA	0.018	0.018	0.407	0.005	0.230
ACETA-01	0.002	0.002	0.002	0.002	0.081
N2	0.765	0.765	0.003	0.790	0.000
O2	0.177	0.177	0.001	0.183	0.000
Mass Flows (kg/hr)	307878	307878	12110	295768	7540

Component Mass Fractions					
ETHANOL	0.008	0.008	0.063	0.006	0.224
WATER	0.017	0.017	0.264	0.007	0.272
CO2	0.006	0.006	0.000	0.006	0.000
CO	0.001	0.001	0.000	0.001	0.000
AA	0.036	0.036	0.668	0.010	0.400
ACETA-01	0.003	0.003	0.002	0.003	0.104
N2	0.734	0.734	0.003	0.764	0.000
O2	0.194	0.194	0.001	0.202	0.000

Table 5: Stream summaries for streams 18-22

Stream Number	18	19	20	21	22
Phase	Liquid	Liquid	Liquid	Mixed	Liquid
Temperature (°C)	40	156	40	40	118
Pressure (bar)	4	3	3	2	2
Molar Vapor Fraction	0	0	0	0	0
Mole Flows (kmol/hr)	549	176	372	372	282
Component Mole Fractions					
ETHANOL	0.097	0.000	0.143	0.143	0.008
WATER	0.530	0.017	0.774	0.774	0.952
CO2	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000
AA	0.337	0.983	0.030	0.030	0.040
ACETA-01	0.034	0.000	0.049	0.049	0.000
N2	0.002	0.000	0.003	0.003	0.000
O2	0.001	0.000	0.001	0.001	0.000
Mass Flows (kg/hr)	19650	10473	9170	9170	5611
Component Mass Fractions					
ETHANOL	0.125	0.000	0.267	0.267	0.018
WATER	0.267	0.005	0.566	0.566	0.861
CO2	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000	0.000
AA	0.565	0.995	0.074	0.074	0.121
ACETA-01	0.041	0.000	0.088	0.088	0.000
N2	0.002	0.000	0.003	0.003	0.000
O2	0.001	0.000	0.001	0.001	0.000

Table 6: Streams summaries for 23, AA, AIR, and FEED streams

Stream Number	23	AA	AIR	FEED
Phase	Vapor	Liquid	Vapor	Liquid
Temperature (°C)	91	50	25	25

Pressure (bar)	2	3	1	2
Molar Vapor Fraction	1	0	1	0
Mole Flows (kmol/hr)	91	176	10203	217
Component Mole Fractions				
ETHANOL	0.562	0.000	0.000	0.997
WATER	0.220	0.017	0.000	0.003
CO2	0.001	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000
AA	0.000	0.983	0.000	0.000
ACETA-01	0.203	0.000	0.000	0.000
N2	0.010	0.000	0.791	0.000
O2	0.003	0.000	0.209	0.000
Mass Flows (kg/hr)	3558	10473	294320	10000
Component Mass Fractions				
ETHANOL	0.660	0.000	0.000	0.999
WATER	0.101	0.005	0.000	0.001
CO2	0.001	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.000
AA	0.000	0.995	0.000	0.000
ACETA-01	0.228	0.000	0.000	0.000
N2	0.007	0.000	0.768	0.000
O2	0.002	0.000	0.232	0.000

Table 7: Stream summaries for fuel gas streams, product stream, recycle stream, and waste stream

Stream Number	FUEGAS2	FUELGAS1	PRODUCT	RECYCLE	WASTE
Phase	Vapor	Vapor	Liquid	Mixed	Liquid
Temperature (°C)	40	40	50	50	50
Pressure (bar)	3	4	2	2	2
Molar Vapor Fraction	1	1	0	0	0
Mole Flows (kmol/hr)	0.2	9998	176	91	282
Component Mole Fractions					
ETHANOL	0.017	0.000	0.000	0.562	0.008
WATER	0.021	0.000	0.017	0.220	0.952
CO2	0.004	0.004	0.000	0.001	0.000
CO	0.001	0.001	0.000	0.000	0.000
AA	0.000	0.000	0.983	0.000	0.040
ACETA-01	0.074	0.000	0.000	0.203	0.000
N2	0.712	0.807	0.000	0.010	0.000
O2	0.170	0.187	0.000	0.003	0.000
Mass Flows (kg/hr)	7	288228	10473	3558	5611
Component Mass Fractions					
ETHANOL	0.026	0.000	0.000	0.660	0.018

WATER	0.013	0.000	0.005	0.101	0.861
CO2	0.006	0.006	0.000	0.001	0.000
CO	0.001	0.001	0.000	0.000	0.000
AA	0.001	0.000	0.995	0.000	0.121
ACETA-01	0.109	0.000	0.000	0.228	0.000
N2	0.664	0.784	0.000	0.007	0.000
O2	0.181	0.207	0.000	0.002	0.000

Results

The following information describes the results of the Aspen model from the given process conditions and specifications above.

Process Narrative

The starting point of the process is the initial raw materials, ethanol and water, entering the process at 25°C and 2 bar. 10,000 kg of these materials at a composition of 99.9% ethanol and 0.01% water enters the process through a mixer, M -101, which is joined by the recycle stream that will be discussed later in the process. From the mixer, the recycle and ethanol/water mixture enters the surge drum, V-101, at a temperature of 38°C and a pressure of 2 bar. The mixture is then taken from the surge drum and pumped to another mixer at 8 bar. Air is also introduced to the mixer at this point. The air stream enters the process at 25°C and 1 bar. To accommodate for the low pressure, the air stream goes through a multistage compressor (C-101 and C-102) with a cooler in between the stages (E-101), as well as two knock out drums to collect excess water that can't enter the compressors. The air leaves the first stage of the compressor at 176°C and 3 bar. Because of the safety risks of air being too hot after a large compression, a cooler was put in between the stages to cool the air stream to 35°C. From the cooler, the air enters the second stage of the compressor and leaves at a temperature of 175°C and 8 bar. This stream then joins the ethanol/water and recycle components in the mixer M-102.

The material exits the mixer at a temperature of 126°C and 8 bar. This enters a heat exchanger, E-102, and exchanges heat with the reactor effluent as the cold inlet stream. This stream is heated to 178°C and exits at a pressure of 6 bar due to pressure drop in the heat exchanger. This stream then enters the reactor R-101. The reactor operates at the conditions of 270°C and 6 bar. Additionally, from the reactions, acetic acid, CO, and CO₂ are now introduced to the process by the reactor effluent stream. This stream, at conditions of 270°C and 6 bar, is cooled by the inlet cool stream from 270°C to 178°C. The effluent then goes through another heater E-102 to further cool the stream to 30°C before entering the flash vessel.

The stream enters the flash vessel, V-201, at 30°C and 4 bar. The flash vessel operates at the same conditions as the incoming stream. This then separates into two streams: the bottoms, which contains a mixture of leftover reactants with very little CO and CO₂, and the distillate, which contains most of the CO and CO₂, along with some of the excess reactants. The distillate then flows through an adsorption column T-201, which is designed to recover 99.9% of the excess reactants, while separating out the CO and CO₂ as a fuel gas stream. Once the excess reactants are purged in this way,

the stream joins the flash tank bottoms in the mixer M-201 at conditions of 40°C and 4 bar. The outlet of the mixer enters the first separation column T-202 at the same conditions.

The first column was targeted to be the separation between the acetic acid product and the rest of the components in the process. The bottoms stream, containing approximately 99.5% acetic acid product, exits the reboiler at 156°C and 3 bar. Because the temperature is unsafe for handling, this was then cooled by a cooler E-204 to 50°C. To achieve a lower pressure for further safe handling, the product stream pressure is reduced to 2 bar by a valve V-2.

The condenser at the top of T-202 contains two streams: the distillate and the fuel gas. The fuel gas stream, mostly containing CO and CO₂, exits the condenser at 40 °C and 3 bar to be scrubbed somewhere downline in the process. The second stream exiting the condenser contains mostly excess reactants and water. Because water aids the unwanted side reactions, the distillate enters a second column T-301 to purge the stream of water and create a wastewater stream. The bottoms, mostly water, exits the column at 118 °C and 2 bar. To further cool the stream for safe handling, another cooler (E-304) was used to cool the stream from 118°C to 50°C.

The distillate of T-301, containing the desired recycle components, exits the condenser at 91°C and 2 bar. Because this stream joins with the raw material stream entering the initial mixer, it is cooled by cooler E-303 to 50°C.

The table below shows the results of the Aspen model.

Table 8: Process Outputs from Aspen Model

Variable	Required	Actual
Acetic Acid Production (kg)	≥10000	10,448.50
Inlet Pressure to HX (barg)	6 to 7	6.88
Air/Hydrocarbons (mol/mol)	35	35.7
Gas Entering Reactor Temp (C)	≥200	220
Effluent CO₂/Acetic Acid ratio (mol/mol)	0.23	0.2299
Effluent CO /Acetic Acid (mol/mol)	0.08	0.08
Adsorber H₂O recovery	99%	99%
Adsorber Acetaldehyde recovery	99%	99%
Liquid waste conditions	1 barg, ≤ 50C	1 barg, 50C
Product stream conditions	1 barg, ≤ 50C	1 barg, 50C

Acetic Acid Purity	$\geq 99.5\%$	99.5%
Product ethanol composition (ppm)	≤ 5	2.74
Product acetaldehyde composition (ppm)	≤ 5	0.00025
Product water composition (wt %)	>0.5	0.005
Acetic Acid column flooding	70%	67.26%, 69.81%
Ethanol column flooding	70%	66.22%

Reactor Steam Generation

Due to the reaction in the reactor being exothermic, the reactor releases heat upon reaction completion. In order to maximize the revenue of the plant, a design was put in place to use the heat generation in the reactor to product low pressure steam. This was modelled by inputting a heat exchanger (E-401) into the Aspen model, and using the produced heat from the reactor as the exchanged heat source. A boiler water line was also inputted as the source of water to be used as steam somewhere else in the plant. The water was sent to the inlet of a flash separator (T-401), where it was separated into condensed steam and liquid water. The liquid water was recycled back into E-401. This system simulates a reactor jacket that produces steam from the heat of reaction.

Equipment Summary

The following table shows a summary of the equipment used in the acetic acid production process. Calculations for the equipment can be shown in Appendix C, and equations used for sizing can be found in the Design of Equipment section in the Discussion.

Table 9: Equipment Summary of the Heat Exchangers used in the Acetic Acid Process Model

Heat Exchangers	
E-101	E-102
A = 539.8 m ²	A = 769.9 m ²
Carbon steel, shell-and-tube design	Stainless steel, shell-and-tube design
Process stream in shell	Process stream in shell
Q = 11756.5 kW	Q = 8531.4 kW
Maximum pressure rating of 3 bar	Maximum pressure rating of 7.9 bar
E-201	E-202
A = 470 m ²	A = 147.6 m ²
Stainless steel, shell-and-tube design	Stainless steel, shell-and-tube design
Process stream in tube	Process stream in shell
Q = 17370.3 kW	Q = 18968.3 kW
Maximum pressure rating of 4 bar	Maximum pressure rating of 3 bar
E-203	E-204
A = 247.3 m ²	A = 11.3 m ²
Stainless steel, shell-and-tube design	Stainless steel, shell-and-tube design
Process stream in shell	Process stream in tube
Q = 19419.2 kW	Q = 438.9 kW
Maximum pressure rating of 10 bar	Maximum pressure rating of 3 bar
E-301	E-302
A = 10.2 m ²	A = 9.8 m ²
Stainless steel, shell-and-tube design	Stainless steel, shell-and-tube design
Process stream in tube	Process stream in shell
Q = 1473.6 kW	Q = 3063.7 kW
Maximum pressure rating of 2 bar	Maximum pressure rating of 10 bar
E-303	E-304
A = 9.2 m ²	A = 5.4 m ²
Carbon steel, shell-and-tube design	Stainless steel, shell-and-tube design
Process stream in shell	Process stream in shell
Q = 1055.5 kW	Q = 431 kW
Maximum pressure rating of 2 bar	Maximum pressure rating of 2 bar

Table 10: Equipment Summary of the Pumps used in the Acetic Acid Production Process

Pumps	
P-101 A/B	P-102 A/B
Centrifugal/electric drive	Centrifugal/electric drive
Carbon Steel	Carbon Steel
Power = 345.9 kW	Power = 205.5 kW
50% efficient	80% efficient
Pressure out = 7.9 bar	Pressure out = 3 bar
P-103 A/B	
Centrifugal/electric drive	
Carbon Steel	
Power = 22.3 kW	
70% efficient	
Pressure out = 2 bar	

Table 11: Equipment Summary of the Compressors used in the Acetic Acid Production Process

Compressor	
C-101 A/B	C-102 A/B
Centrifugal/electric drive	Centrifugal/electric drive
Carbon Steel	Carbon Steel
Compressor Rating = 1.73	Compressor Rating = 1.63
Number of Stages = 2	Number of Stages = 2
Pressure out = 3 bar	Pressure out = 8 bar
Efficiency 72%	Efficiency 72%
Net work = 12583.5 kW	Net work = 11693.1 kW

Table 12: Equipment Summary of the Vessels used in the Acetic Acid Production Process

Vessels	
V-101	V-102
Vertical	Horizontal
Stainless Steel	Carbon Steel
Length = 6.59 m	Length = 1.86 m
Diameter = 3.30 m	Diameter = 0.62 m
Maximum pressure rating of 1.9 bar	Maximum pressure rating of 1 bar
V-103	V-201
Horizontal	Horizontal
Carbon Steel	Stainless Steel
Length = 1.86 m	Length = 12.66 m

Diameter = 0.62 m Maximum pressure rating of 3 bar V-202 Horizontal Stainless Steel Length = 4.18 m Diameter = 1.39 m Maximum pressure rating of 3 bar V-301 Vertical Stainless Steel Length = 2.59 m Diameter = 0.86 m Maximum pressure rating of 2 bar	Diameter = 4.22 m Maximum pressure rating of 4.1 bar V-401 Vertical Carbon steel Length = 1.95 m Diameter = 0.65m Maximum pressure rating of 12 bar
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Table 13: Equipment Summary of the Pumps used in the Acetic Acid Production Process

Reactor R-101 Stainless steel, Jacket non-agitating 15337 tubes OD = 0.025 m L = 6 m

Table 14: Equipment Summary of the Towers used in the Acetic Acid Production Process

Towers T-202 Stainless Steel 25.17 m packing 25 mm metal intalox packing D = 2.95 m , D = 4.15 m Max pressure rating: 4 bar	T-301 Stainless Steel 9 SS sieve tray stages 0.8 m tray spacing D = 0.97 m Max pressure rating: 3 bar
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Utility Summary

The table below shows the results of the required utility usages for each of the heat exchangers.

Table 15: Utility Summary for Heat Exchangers in the Aspen model

E-101	C-101	C-102	R-101	E-201	E-202
CCW	ELEC	ELEC	STMGEN	CCW	LPS
1010500	9060	8419	48101	1492830	34629

E-203	E-204	E-301	E-302	E-303	E-304
CW	CW	CW	LPS	CCW	CW
1631690	38025	126319	5444	90112	36953

*All are in kg/hr except the ELEC components which are in kW

Column Profiles

The following figures depict the composition, temperature, and hydraulic profiles of each of the designed columns.

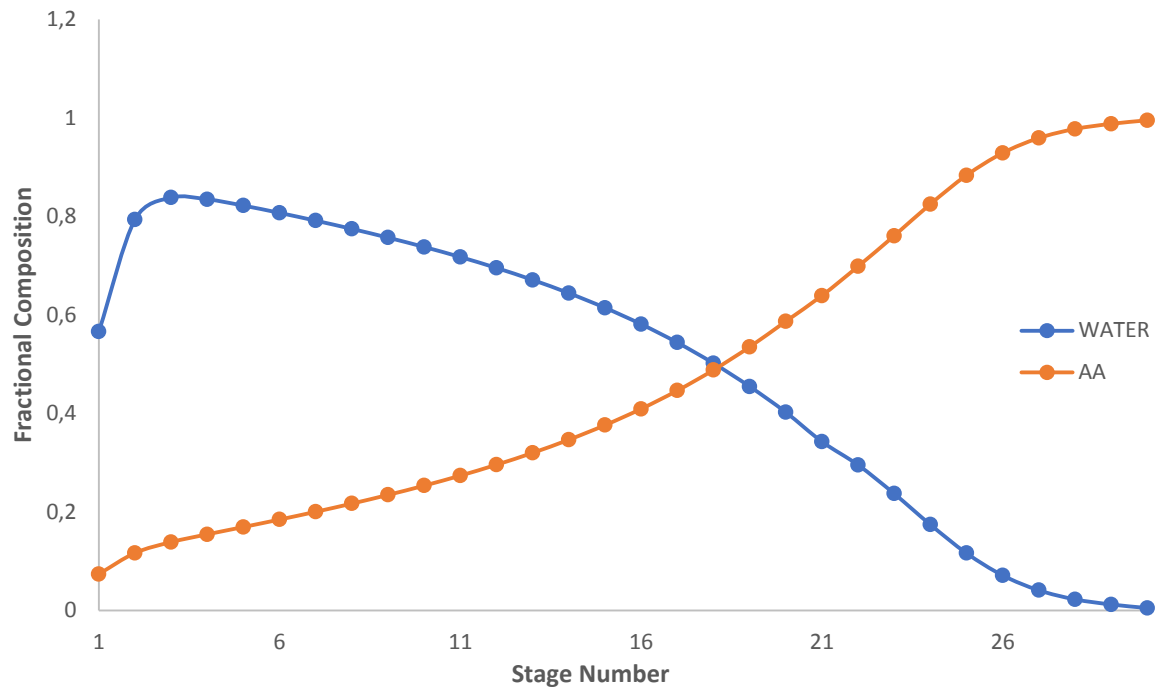


Figure 1: Composition profile of the Acetic acid - water column T-202

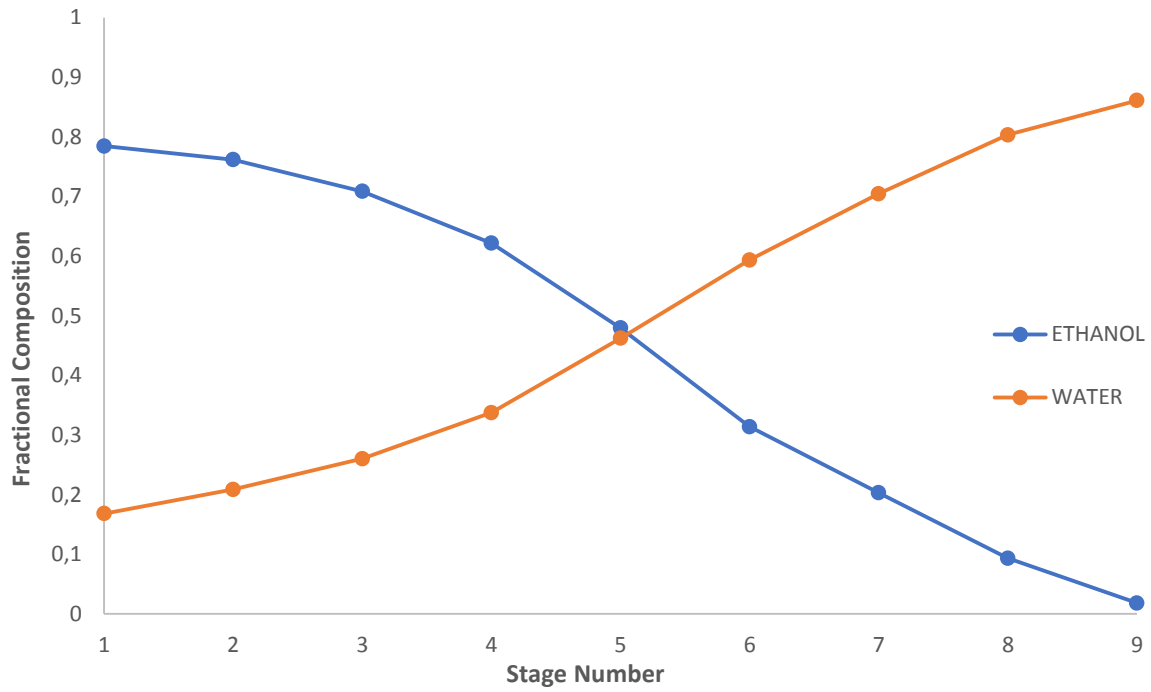


Figure 2: Composition profile of the ethanol-water column T-301

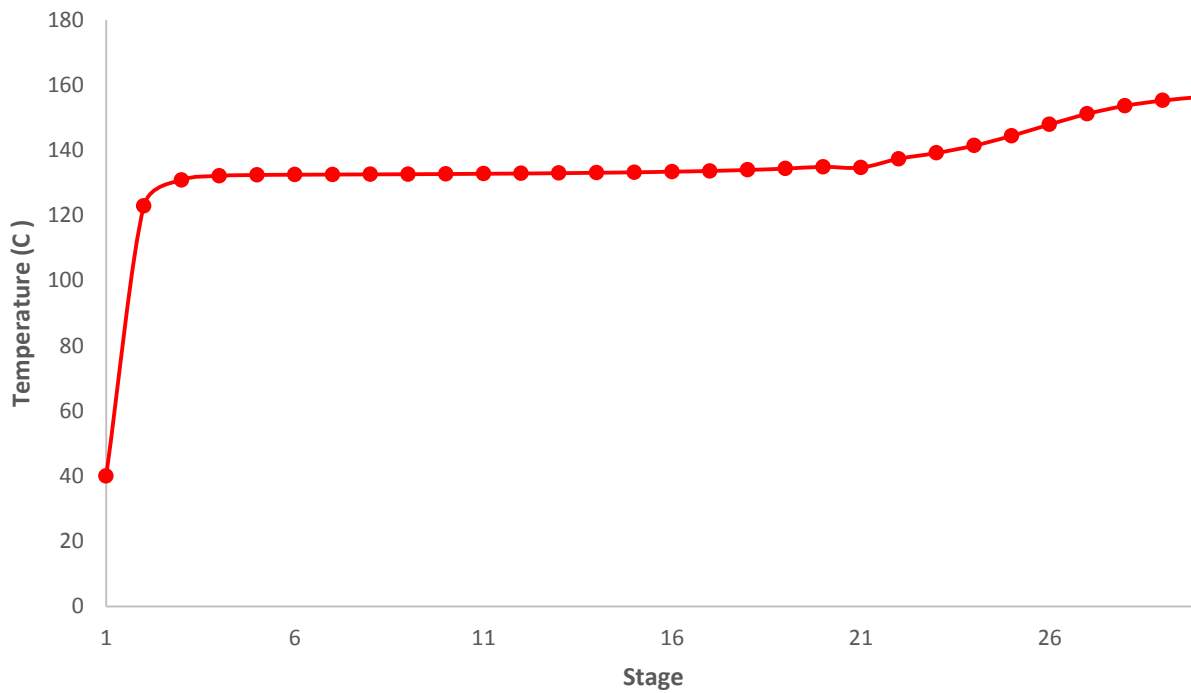


Figure 3: Temperature profile of the Acetic acid - water column T - 202

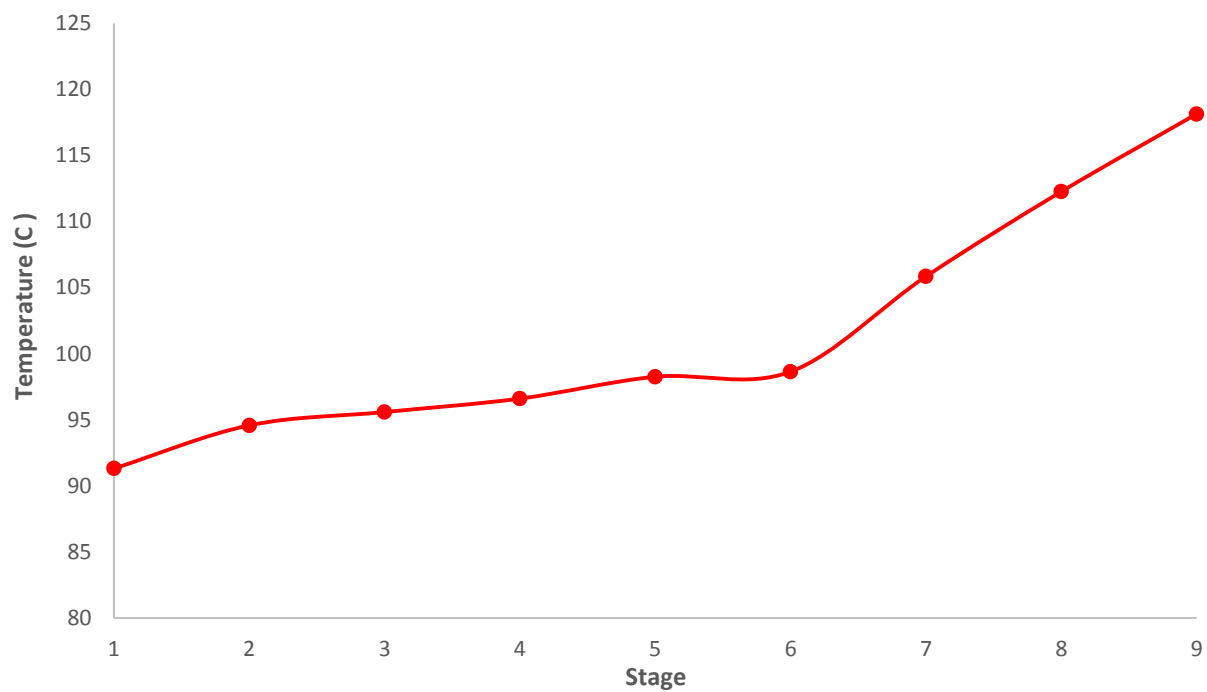


Figure 4: Temperature profile of the water - ethanol column T-301

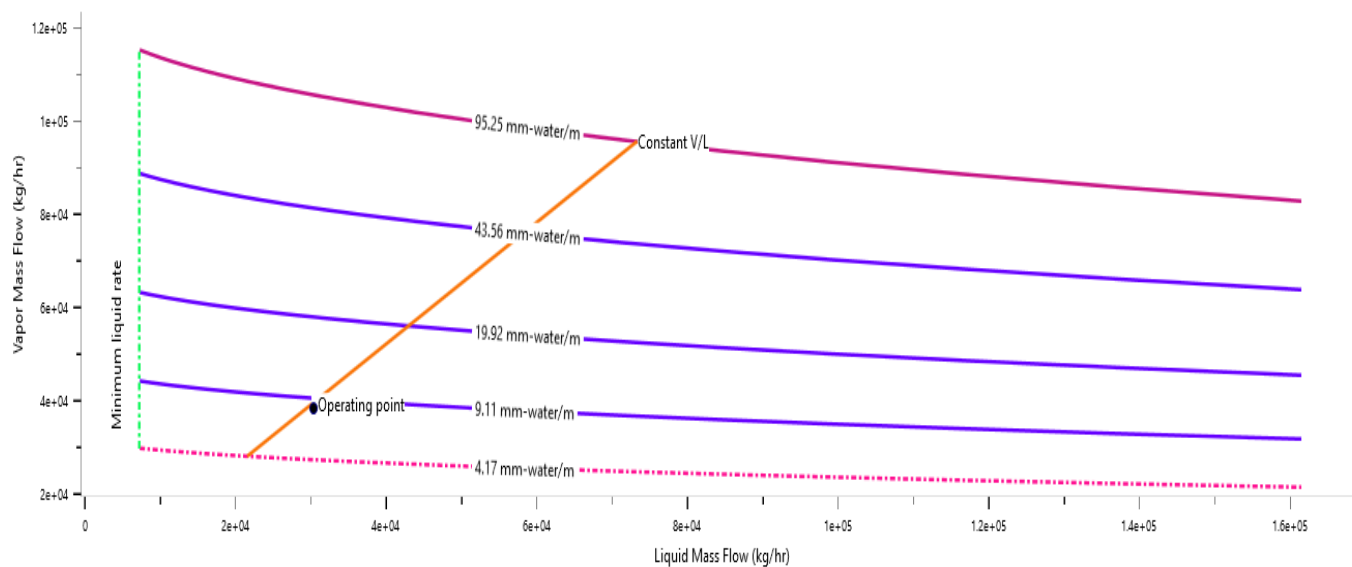


Figure 5: Hydraulic plot for the AA/water column at stage 10, D = 2.95 m

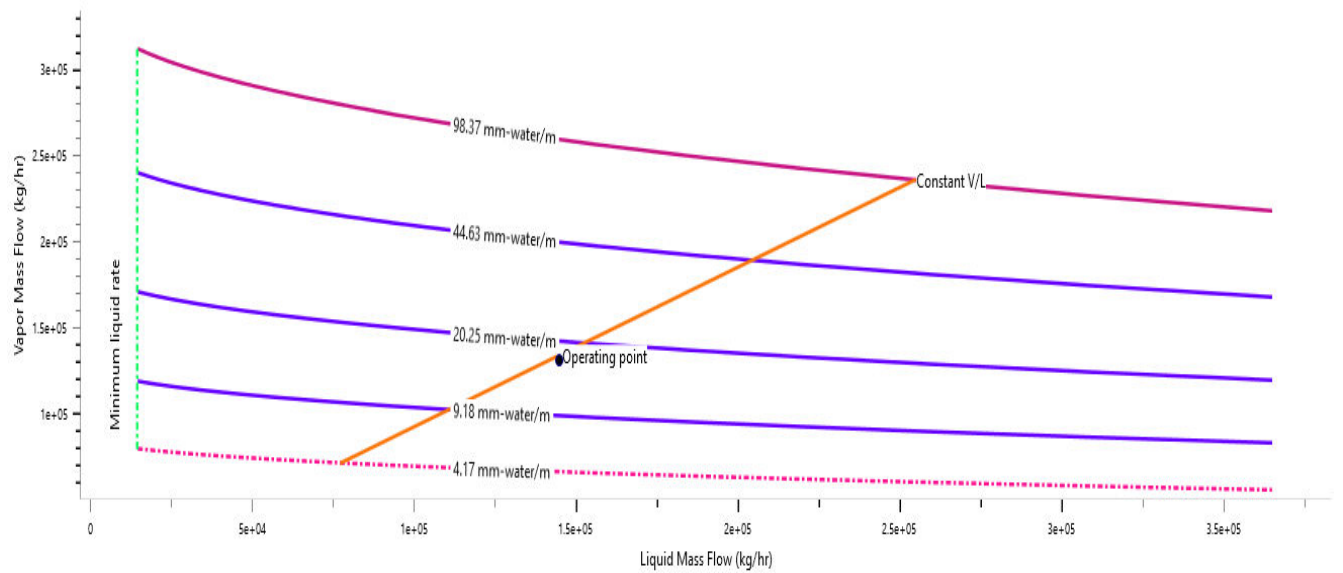


Figure 6: Hydraulic plot for the AA/water column at stage 26, $D = 4.15$ m

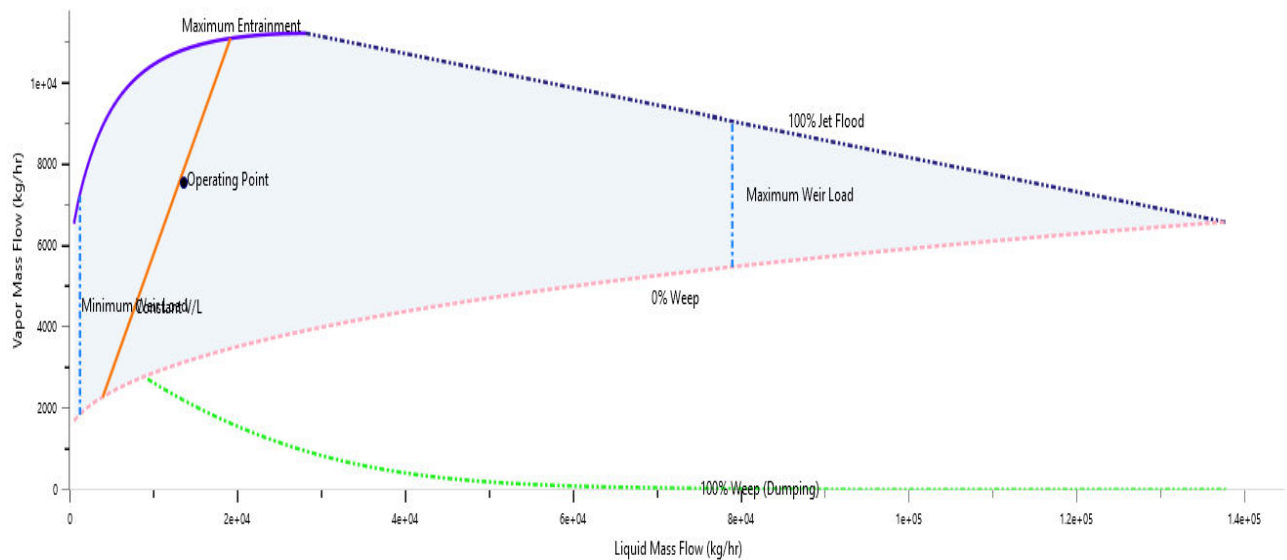


Figure 7: Hydraulic plot for the Ethanol/water packed column at theoretical stage 6, $D = 0.97$ m

Discussion

The following sections discuss the results found from the Aspen model for design justification, equipment design, thermodynamic package, and cost analysis.

Thermodynamic Package Justification

In order to find the best thermodynamic package for the model data, a few different packages were tested against experimental data to find which modelled the data the most accurately. The models tested were NRTL, Wilson, UNIQUAC, and SRK. SRK is a cubic equation of state, which NRTL, Wilson, and UNIQUAC are activity coefficient based models. The experimental data was found using the NIST tables provided in the Aspen software. The thermodynamic model was chosen based on first deciding the best model for the ethanol/water separation, and then the acetic acid/water separation. The second column was modelled first because it is the most complicated separation due to the existing azeotrope.

The model was originally run in NRTL to start the model. After the specifications for the process design were met, the thermodynamic models were compared against the experimental data given in NIST. After researching different data, it was found that there was not data given at the exact pressure that the separation columns were running at. The ethanol/water column was specified to run at 2 bar; however, the closest experimental data was at 2.8 bar, so this data was used after being determined it was close enough to the process specifications. The acetic acid/water column was specified to be at 3 bar; however, the closest experimental data was at 2.7 bar, so this data was used instead. A T-xy diagram was made using the NIST data, as well as the data for the tested models at 2.8 bar. The figure below shows these comparisons for the ethanol/water separation.

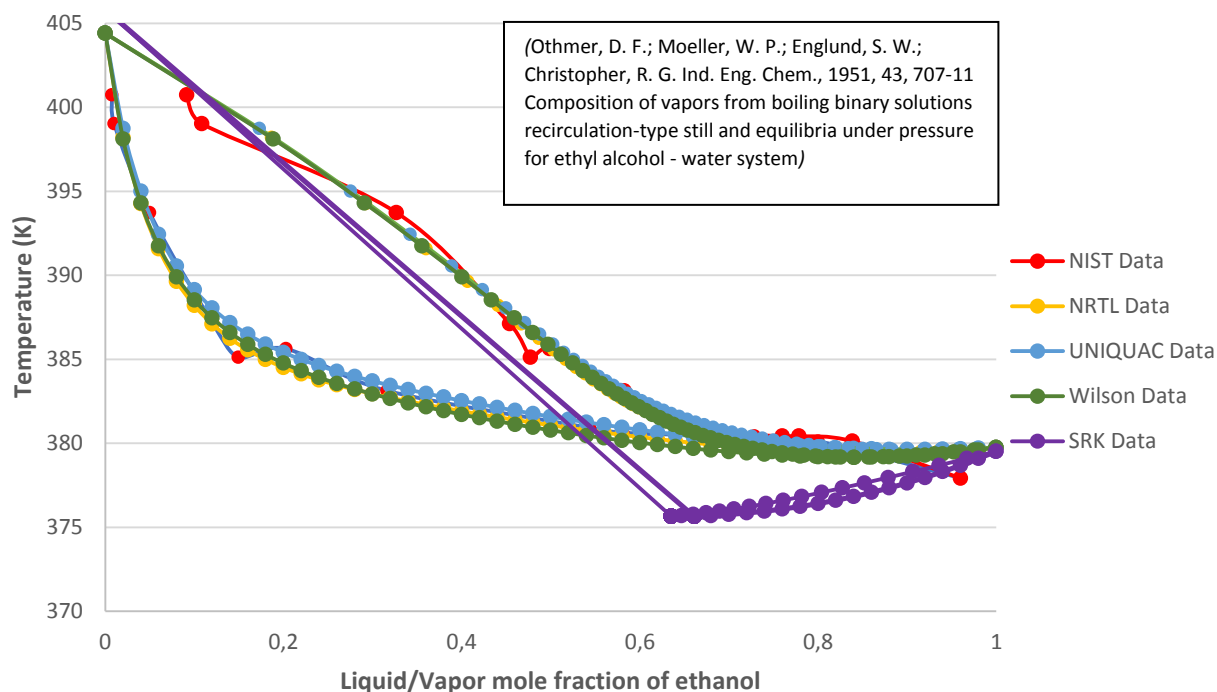


Figure 8: Ethanol/water Txy diagram at P = 2.8 bar

From the figure, it can be seen that SRK does not fit the NIST data. This is because cubic equations of state are known to not be accurate when it comes to non-ideal separations, especially those that have azeotropes. For this reason, SRK was ruled out. The remaining data for the activity coefficient based models all had a relatively close trend to that of the NIST data. Looking at the figure, the UNIQUAC data for the liquid line is almost exactly similar to the NIST data and the rest of the data; however, the vapor line is slightly above the NIST data, so for this reason, it was ruled out.

With Wilson and NRTL remaining, further research was done on thermodynamic modelling. It was found that NRTL was the final choice for the package due to being an extension of the Wilson equation, and therefore, being a more accurate choice. As stated previously, it is important to note that the above data is at slightly different conditions than used in the process. The next figure shows confirmation that NRTL is the correct choice for the acetic acid/water separation as well.

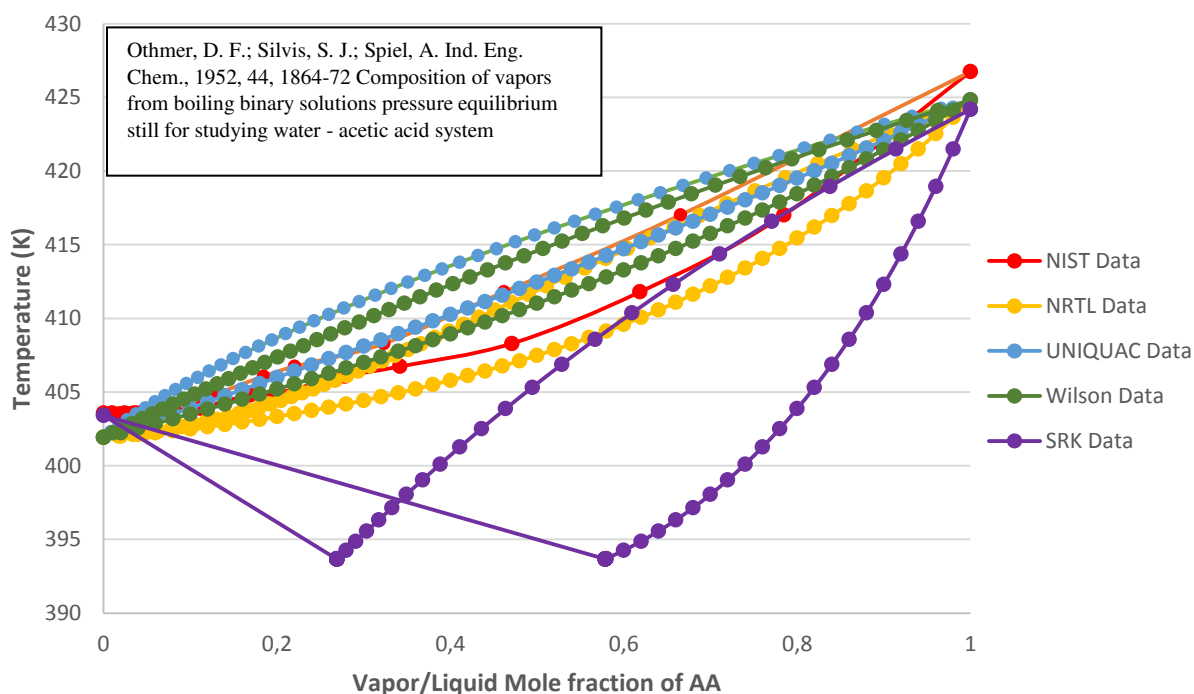


Figure 9: Acetic acid/water Txy diagram at P = 2.7 bar

Process Design Justification

Literature and previous designs were researched before preliminary design began. The most common method of acetic acid production was using methanol carbonylation. Though this

method is widely known and continues to be researched, the method specified to the chemical engineering team was the dehydrogenation of ethanol. The reactor was specified as having 6 m length tubes with an inner diameter of 25mm with conversions of acetaldehyde of 92% and ethanol to 80%.

Air was used as the oxidant for this reaction, given that it is a cheap utility and easy to obtain. The air was sent to the reactor on the basis that there would be 35 mol/mol for air/hydrocarbons to prevent any safety hazards. The air was compressed by using a multi stage compressor, modeled by two compressors and a cooler in between. The engineering group decided to use a multistage compressor versus one because the air would become too hot after being compressed from 1 bar to 5 bar in one step, and could cause a safety concern. With the multistage compressor, the air can be cooled in between, and then compressed again. The cost was determined to be worth the safety adjustment.

From the reactor, it was determined that the fuel gas created in the side reactions should be separated out first, given that it is the easiest separation. This was done by using a flash vessel versus a column, because the separation was easy to accomplish in minimal stages due to the large gap in boiling points between the gases and the rest of the components in the separation. It was also less expensive than another column, so capital costs are saved by using the flash vessel.

An adsorption column was determined to be used to maximum recovery of the excess reactants, acetaldehyde and ethanol. This was modelled by separation block in Aspen. From the flash vessel, two options were explored: separating out the waste water from the rest of the components first, or separating the excess reactants from the feed first. The second option was tested first. The column was designed to separate the excess components from the acetic acid and water. After running the column initially in equilibrium, it was determined to be difficult to separate the excess reactants out due to the azeotrope that exists between water and ethanol. Because no further separation could be done after the azeotrope, the amount of ethanol left in the bottoms was too much and would cause impurity in the end product stream because the ethanol was larger than 5 ppm. It was determined that the end product specifications could be done in this way; however, the number of stages and height of the column proved to be impractical for design due to being too high.

Because of the difficulty of the initial excess reactants separation, the option of separating the water first was tested. This proved to be an easier separation because the ethanol that wasn't separated was sent to the waste water stream instead of the end product. Each gas column was equipped with a fuel gas stream to prevent CO₂ and CO from entering the end product and waste water streams.

The excess reactants are sent to a recycle back into the reactor to save money on raw materials, which is further reacted with air to product more acetic acid.

Design of Equipment

Columns

The first column, T-202, was designed to be a packed column operating at a pressure of 3 bar and with 30 theoretical stages of packing. The theoretical feed stage was determined to be above stage 21. The feed stage was determined by examining the composition plots and placing the composition of the feed stream at the stage that fit the plot. These plots can be seen in the Results section. The packing is 25 mm metal intalox packing.

The columns were designed by first running the assumptions and first stage guesses in Aspen under Equilibrium conditions in order to get an initial idea of what the column diameters would be. Next, the columns were run in Rate – Based, which assumes that the equilibrium stages were not 100% efficient. The diameter was then changed by the user based on what the hydraulic plots looked like and what the flooding percentage was in various parts of the column. If there was flooding in parts of the column, the diameter was increased.

After running the rate-based method in Aspen, the average height per theoretical stage was determined to be approximately 0.839 m for a total of 23.492 m for the stages plus 8 extra meters for the intermediate packing support. The sump for T-201 was calculated to be 1.20 m, and the sample calculation for this can be found in Appendix C. The total height for the packed column is 32.692 m. The height per stage diagram for the packed column can be found in Appendix A. reflux ratio of 3 was determined to be the optimal point of water to acetic acid separation, and resulted in greater recovery of acetic acid in the DSTW model used as preliminary modeling. The bottoms to feed ratio was determined to be 0.321 based on Aspen's calculation and iterations performed to find the optimal conditions for an acetic acid purity of 99.5% or greater.

The column was targeted to be at an average of 70% flooding at all times. This was modelled by creating a design specification for the software, and the appropriate diameters were found in this way. The hydraulic plots for each of the diameters calculated for this column show that it is operating a safe point. These plots can be found in the Results section.

The top half of the column, stages 2 – 22, has a diameter of 2.9502 meters and a flooding approach of 67.26%. The bottom half of the column, stages 23-29, has a diameter of 4.1457 m and a flooding approach of 69.82. The bottom half of the column has a larger diameter due to the amount of liquid in the bottom versus the top. Because of the larger composition of liquid, the bottom of the column is more prone to flooding, and therefore, a larger diameter is required to stay in the 70% range. The hydraulic plots for both sections of the column are shown in the Results section.

The second column, T-301, was designed to be a trayed column operating at a pressure of 2 bar with 9 stages and a feed stage on tray 6. Once again, the feed stage was determined by examining the composition plot and placing the composition of the feed stream at the stage that fit the plot the best. This plot can be found in the Results section. The column was designed in the same way as the first column: first running the Aspen software in Equilibrium to get an initial idea of the diameter, and then changing the diameter slightly upon using Rate-Based.

After running the rate based method in Aspen, the average efficiency of each tray was determined to be 14.7 %. The efficiency per tray results can be found in Appendix A. The height of the column was determined to be approximately 5.6 m plus 1 extra meter for the height above the top tray. A sump of height of 1.63 was added to the bottom of the column for a total of 8.23 m after calculating the diameter of the column to be 0.971 m.

The column was targeted to be at an average of 70% at all times; the column design resulted in being around an average of 66.23% flooding. The hydraulic plot for this column in the Results section shows that it is operating at optimal conditions. A reflux ratio of 1.5 was used for this column as the optimal point of ethanol and acetaldehyde recovery to the recycle stream. The distillate to feed ratio was determined to be 0.243 by Aspen to calculate a water composition of 10% in the distillate recycle to improve separation of the ethanol and water. The hydraulic plots for the trayed column are shown in Results Section.

Reactor

The reactor used in this process design is a multi-tube quasi-isothermal fixed-bed reactor with the catalyst contained in the reactor tubes. The tubes are 6 m in length with an outer diameter of 25 mm and a wall thickness of 0.003 m. The heat generated by the reactors is used to create steam that can be used elsewhere in the plant. This is modelled as a heat exchanger and flash tank by the Aspen software. The heat from the reactor is used as the heat source in the model heat exchanger and shows the steam coming out as the output of the flash tank. In order to design the reactor, it was necessary to calculate the pressure drop across the tubes. Because the surface area of the inner tube was known, the diameter and size of the reactor was able to be calculated. This was done by the following equations, and the sample calculation can be shown in Appendix C.

The first equation shows how to find the surface area of the inner tube.

$$SA = \pi * \left(\frac{d_0 - wall\ thickness}{2} \right)^2$$

Where:

SA = surface area of the inner tube

d_0 = inner diameter

From the surface area, the volume of a single tube could be found by multiplying by the length of the tubes.

$$V = SA * L$$

Where:

V = volume of a single tube

L = tube length

Once the volume was known, the volumetric flowrate going into the reactor was divided by the volume of the tubes in order to get the total number of tubes required for the reactor.

$$N = V_{flow}/V_{tube}$$

Where:

N = number of tubes required in the reactor

The number of tubes is necessary to calculate the pressure drop through the reactor. The pressure drop was estimated by the Ergun Equation by knowing the number of tubes and other physical properties of the material going through the reactor.

$$\Delta p = \frac{150 * \mu L}{D_p^2} * \frac{(1 - \epsilon)^2}{\epsilon^3} v_s + \frac{1.75 L \rho}{D_p} * \frac{1 - \epsilon}{\epsilon^3} v_s^3$$

Where:

p = pressure

D_p = diameter of the catalyst

μ = viscosity

ϵ = void fraction

v_s = superficial velocity

ρ = density

The pressure drop was found and modelled in the Aspen system using a pinch valve. Note that this valve is not part of the actual design, it is merely a way to simulate the pressure drop of the reactor in the Aspen system.

As stated in the process narrative, a steam regeneration system was modelled in order to simulate steam being generated from the reaction heat release. From this model, approximately 48,225.3 kg of hour can be generated from the heat released by the reactor. This steam can be used elsewhere in the plant and is shown in CAPCOST as excess revenue. This will be discussed later in the report.

A couple of catalysts were researched for this type of reactor and acetic acid production method. One of which was mentioned earlier, which is an iridium based catalyst. This was shown to reduce the side reactions of acetic acid into CO and CO₂. Another catalyst researched was a platinum based catalyst. This has the advantage of being slightly cheaper than an iridium catalyst; [3] however the iridium can reduce reactant waste. It is recommended that further research is done on what type of catalyst is used in this process, should it be decided to move forward with this design.

Heat Exchangers

The heat exchangers used in the Aspen model were all modelled using the EDR feature in the software. The sizing of the heat exchangers were generated by inputting the material of the heat exchanger, the type of flow through the heat exchanger, and the location of the hot flow for each of the heat exchangers. The results of EDR also showed the pressure drop through the

exchangers. The results from the EDR analysis can be shown in Appendix A. The size calculation produced by the software was used to price the exchangers using CAPCOST, which will be discussed later in the report.

Flash Separators

The calculation of the flash separators used in the process followed the Souders-Brown equation from Turton [4]. The gas velocity in the gas/liquid separator was used to size the separator based on the drop settling condition. The equation below is the Souder-Brown equation and it is used to find v_{max} . From heuristics, good performance of the velocity is from 30%-100%. For the actual velocity used, v_{max} was multiplied by 75%.

$$v_{max} = K_{Derated} \sqrt{\frac{\rho_l}{\rho_v} - 1} \quad (1)$$

Where,

v_{max} = maximum velocity through demister (m/s)

K = Constant that is de-rated at elevated pressures

$K_{Derated}$ = derated based on GPSA Engineering Data Book, 11th edition

ρ_l = density of the liquid stream phase (kg/m³)

ρ_v = density of the vapor stream phase (kg/m³)

$$v = 0.75v_{mas}$$

Where,

v = actual vapor velocity (m/s)

Once v_{max} is calculated, the diameter can be found assuming the cross-sectional area of the vessel is assumed to be rectangular. Assuming a rectangular cross-sectional area implies that the vessel is horizontal. A horizontal vessel allows for the maximum amount of vapor to be separated via mass transfer. The diameter of the flash separator was calculated by Equation (2) below.

$$D = \sqrt{\frac{q_v}{(v\rho_v \frac{L}{D})}} \quad (2)$$

Where,

D = Diameter of the separator (m)

Q_v = vapor flow (kg/s)

V = vapor flow (m/s)

ρ_v = density of the vapor stream phase (kg/m³)

L/D = length to diameter ratio for optimal volume of vessel

The sample calculations for the flash separators can be found in Appendix C.

Pumps

The pumps were sized by using heuristics in Turton [4] to calculate the required operating power. The power of the pump can be calculated by equation (3) below.

$$P = \frac{1.67q\Delta P}{\epsilon} \quad (3)$$

Where,

P = operating power (kW)

q = liquid flow (m³/min)

ΔP = change in pressure (bar)

ϵ = efficiency

If there is no change in height of the pipeline, then ΔP is found by the difference of inlet and outlet pressures. If there is a ΔP due to a height change, then ΔP can be found by equation (4).

$$\Delta P = \rho g \Delta H \quad (4)$$

Where,

ρ = density (kg/m³)

g = gravity (m/s²)

ΔH = column height

$$\Delta H = 2N + 10 \text{ (ft)}$$

Where,

N = number of trays

The sample calculations for the pump heuristics are shown in Appendix C.

Air Compressors

The air compressors that were used in the process were designed by using Turton's heuristics [4]. The compressor rating was determined by equation (5) below.

$$CR^N = \frac{P_n}{P_1} \quad (5)$$

Where,

CR = Compression Rating

N = number of stages

P_n = Final pressure (bar)

P₁ = Entering pressure (bar)

The air compressors were designed using Aspen software. The efficiency was assumed to be 72%, and the mechanical efficiency was assumed to be 100%. It is important to note that if the mechanical efficiency was less than 100% in reality, the compressor would be approximately 10% larger. The sample calculations for the compressor rating can be found in Appendix C.

Vessels

The vessels with liquid inlet flows were sized by equation (6) below. The vessels that contain both liquid and vapor were sized by the using Souders-Brown equation as described above for the flash separator calculations. The liquid-holdup time was estimated to be the time at which the vessel is half full to when the liquid is pumped out. The diameter of the vessel can be found by equation (6).

$$D = \sqrt[3]{\frac{V4}{\pi \frac{L}{D}}} \quad (6)$$

Where,

D = diameter (m)

V = volume of tank (m³)

L/D = length to diameter ratio for optimal volume of vessel

Process Controls

Defining process controls for the production of acetic acid was an important step in developing a flexible, safe, optimized process. The chemical engineering team used a variety of control strategies including feedback, split range, and cascade control.

Feedback Control

Process industries heavily rely on feedback control, and consequently feedback control was frequently used in the process design. Feedback control is a closed-loop system that responds to deviations from a given setpoint, responding to a produced error signal. The error signal is the difference between the process variable and the setpoint. Therefore, it communicates how far away the output is from the desired value. Feedback control adjusts a process parameter in response to a deviation to bring the error signal to zero. This control strategy is implemented in multiple level control systems in the design – V-102, V-103, V-201, T-401 - as well as the pressure control for T-201, T-202, T-301 and streams 12 and 20. Feedback control is also implemented in combination with other controllers – yielding Cascade Control.

Cascade Control

When two or more controllers work together to improve response, it's called Cascade Control. Combining controlled variables increases responsiveness because some variables are more reactive than others - e.g. changing a process flow rate will occur faster than changing a vessel temperature [5]. This control strategy is implemented in R-101, cascading control of pressure and temperature of the reactor with the flow rate of the reactor feed. Additionally, temperature control of the distillation columns T-202 and T-301 are cascaded with their respective bottoms flow rate, and the column reflux drum levels are cascaded with the reflux flow rates. Specifically at the recycle stream after T-301, a combination of feedback-feedforward cascading control was implemented to provide both pressure and flow control.

Split Range Control

Split Range Control is commonly used for multistage compressors, and thus was implemented during the air feed preparation step in the design [5]. Two pressure transmitters were placed after their respective knock out drums, and share the same controller on the air inlet stream. This strategy was implemented because while there are multiple stages in the design, there is ultimately one output variable – air feed pressure [6].

Ratio Control

Ratio control is a specific type of feedforward control that maintains the ratio of two process variables at a specified value [7]. Achieving an ideal feed-air ratio before the reactions take place is a crucial step in optimizing acetic acid production – therefore ratio control of streams 3 and 10 was implemented to hold the feed-air ratio at an optimum value.

Safety and Environmental Analysis

The proposed design for the production of acetic acid manages multiple hazardous materials, which are listed along with potential hazards in Table 16.

Table 16: Hazards of the Materials Used

Flammable	Carcinogenic	Corrosive	Asphyxiant
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Ethanol	x		
Acetaldehyde	x	x	
Acetic Acid			x
Carbon Dioxide	x		x
Carbon Monoxide	x		x

Flammability is a major safety concern with the proposed materials in the acetic acid production process. Ethanol, carbon dioxide, carbon monoxide, and acetaldehyde are flammable in the presence of sparks and open flames, and can lead to explosions given a vapor release [8]. In addition to being flammable, the acetic acid product is also highly corrosive, but is not corrosive in the presence of stainless steel (319), justifying the use of stainless steel equipment throughout the process design. Acetaldehyde, a known carcinogen and possible teratogen, is also created as an intermediate step in the process. It is hazardous in many forms including ingestion and inhalation, and repeated exposure leads to organ damage [9].

Process vessels, reactors, and columns include relief valves and rupture disks to combat high pressure release scenarios. Relief systems should send materials to appropriate knockdown drums due to the materials' high flammability. In addition to the drums, vapors should be sent to a flare to prevent high concentrations of explosive gases and vapors [10]. Additionally, isolation valves should be implemented to ensure safe shutdowns for turnover and other maintenance needs. Implementing procedures to avoid ignition sources around the process is imperative – creating designated smoking locations away from plant processes and minimizing electronic devices used around the process are two examples.

Hazardous process conditions in the design include a reactor effluent stream of 270°C, which is quickly cooled in an exchanger, and utilities processes operating at 12 bar to create low pressure steam. General recommendations for safety measure include insulating equipment used for high temperature materials to avoid contact with workers, and safe material storage procedures. Storage of materials, especially waste materials, should be in well ventilated areas, protected from sunlight, and secured [10].

The production of acetic acid from ethanol creates various impurities such as carbon dioxide and carbon monoxide. These materials pose multiple environmental concerns, but the relatively small quantities facilitate manageable conditions from an environmental perspective. Carbon monoxide and carbon dioxide contribute to atmospheric greenhouse gasses, affecting ozone concentrations and further advancing global climate change [11]. As implemented in the design, the use of a flare will greatly counteract these pollutants.

Another environmental concern is the presence of acetic acid in wastewater. The removal of acetic acid is very important due its corrosiveness and negative effects to plants, animals, and aquatic life. The use of activated carbon or fly ash is necessary in wastewater treatment facilities to remove the acetic acid [12].

Cost Analysis

One of the goals of the chemical engineering team was to not only design a process that yields acetic acid in a safe way, but also to keep operating and plant costs down as low as possible. In order to optimize cost, the team considered things such as cheaper materials, lower operating pressures, smaller equipment, and lower operating temperatures.

The total cost of the plant was found by using the CAPCOST excel calculator. Each piece of equipment was entered into the equipment summary portion of the spreadsheet after determining the sizes using heuristic equations. The operating pressure was also used to determine pricing. In order to size equipment safely, the columns and vessels were priced at 1 bar above the operating pressure. The heat exchangers were sized using Aspen EDR analysis. From the EDR results, the pressures were put into the CAPCOST spreadsheet along with material and size.

In some cases, the equipment required for the process was larger than the allowed maximum input into CAPCOST. To get around this situation, the Six Tenths rule was used to price larger equipment. This entails using a ratio using the price of smaller equipment to size the larger equipment. The price was then overrode in CAPCOST to accurately determine the total equipment costs. This is shown below in equation (7).

$$C_{P,2} = C_{P,1} \left(\frac{S_2}{S_1} \right)^n \quad (7)$$

Where,

$C_{P,1}$ = original cost of item

$C_{P,2}$ = new cost of item

S_1 = size of the original item

S_2 = size of the new item

n = economy scale (assumed $n = 0.6$)

The individual utility cost table can be found in Appendix B. These were calculated based on the prices in the following table.

Table 17: Utility Prices used in CAPCOST Analysis

Utility	Price
Electricity	\$0.06/kWh
CW	\$12/cubic m
CCW	\$150/1000 cubic m
LPS	\$8/dekatherm
Generated LPS	+ \$8/dekatherm

The steam generated by the reactor was credited towards the overall COM cost before calculating the cost of production per kg of acetic acid. For this calculation, it was assumed that 12 operators would be needed for this process. The value given in CAPCOST was only for three operators, so this value was multiplied by 3 and is shown in the table below under the Cost of Operating Labor section. The operating hours was assumed to be 8332 hours per year. The operating cost/ kg AA/ y was determined by the equation below.

$$\frac{\$}{kg} \text{ Acetic acid} = \frac{(\text{Annual Utility Cost} + \text{Operating Labor Cost} + \text{Raw Material Cost} - \text{Excess Acetic Acid Credit})}{(\text{kg acetic acid} \frac{\text{acid}}{\text{hr}} * \text{operating hours})} \quad (8)$$

The capital cost in terms of dollars / kg/ year was also calculated by dividing the equipment fixed costs by the recovered acetic acid, which was 10,448.5 kg/ hr.

The following table shows the results from the CAPCOST analysis.

Table 18: CAPCOST Results

Cost Analysis	Cost	Cost (\$/kg AA/y)
Equipment Costs	\$ 23,468,004.00	\$ 0.28
Total Bare Module Cost	\$ 19,200,000.00	\$ 0.23
Grass Roots Cost	\$ 24,600,000.00	\$ 0.30
Cost of Manufacturing (COMd)	\$ 53,785,800.00	\$ 0.65
Annual Operating Costs	\$ 43,806,351.00	\$ 0.53
Raw Material Costs	\$ 37,411,551.00	\$ 0.45
Annual Utility Costs	\$ 5,760,000.00	\$ 0.07
Cost of Operating Labor	\$ 634,800.00	\$ 0.0076
Credit for Excess Acetic Acid Production	\$ 2,163,778.00	\$ 0.5497
Operating Cost (\$/kg/y)	\$	0.50
Capital Cost (\$/kg/y)	\$	0.27

Conclusion and Recommendations

The chemical engineering team was tasked with recovering at least 10,000 kg/hr of acetic acid from 10,000 kg/hr of ethanol and water. The required product must be at least 95% pure with less than 5% water remaining in the stream. The team accomplished this task by sending the stream to the beginning of the process and mixing it with air that had a ratio of 35 mol/mol for air/hydrocarbons to prevent an explosive environment. The mixture then went to the reactor where an exothermic conversion of ethanol to acetic acid occurred. From the energy released, 48,944 kg/hr of steam was able to be produced and credited to the overall process cost. From the reactor, the products and excess reactants were sent through a flash tank to separate the CO and CO₂ in order to get a purer product at the end of the process. To recover the excess reactants, the stream then went through an adsorption column, and then two distillation columns to retrieve pure acetic acid, a waste stream, and a recycle stream for further conversion. By this process, the team was able to recover approximately 10,448 kg/hr of acetic acid with a purity of 95%. The recovery was calculated to be approximately 94% with a selectivity of 81%.

From these results, the process can potentially work as a means of producing over 10,000 kg/hr with 95% purity. The process conditions are never at dangerous pressures or too high or low of temperatures. Multiple control systems were put in place to act as a barrier for any wavering in the process conditions. Though the basic requirements of the process were met, the cost of the process was shown to be too expensive, with the average operating cost/kg AA being about \$0.50/kg AA.

The engineering team recommends that this process is not pursued until further reduction of cost can occur. As seen in the CAPCOST analysis, the most expensive part of the process is the multistage compressor used to pressurize the air stream before meeting with the raw material stream. This was done in two stages with a cooler in between so that the air stream would not become overheated. Due to the large pressure increase of the air stream, the compressors were required to be massive in size and energy consumption, making the utility and bare module costs of the process to be expensive. The team recommends that the two stages are broken down into four or more stages in order to decrease the size and energy consumption of this part of the process. This would also decrease the driver cost.

Further discussion the utility usage, the team would recommend that less of the chilled water is used, and that the cooling water is used instead. This could be done in multiple ways, one of the most prominent is to use multiple coolers and heater to change the temperatures on the stream. If the coolers and heaters were smaller, and were processing smaller changes in temperature, the cooling water would be sufficient, and would therefore reduce the costs of the chilled water utility. For example, in the process, the reactor effluent temperature was cooled from 178 C to 30 C, which is a huge change in the temperature. It is obvious that this heating system required the use of the chilled water. If this cooler were broken up into, say, two or three coolers, the use of

chilled water may be eliminated. Though it is more expensive to buy the equipment up front, it will most likely save costs in the long run due to the annual cost of chilled water being so high.

Another recommendation from the team is to increase the efficiency of the columns. Though the packed column efficiency is relatively high compared to the trayed column, it is still an expensive method of separation due to the packing. The trayed column reached an average efficiency of approximately 14%, which makes for a very tall and expensive column. The team recommends that a sieve tray is used in place of the two columns in order to reduce wasted column space due to low efficiency. Though this is initially expensive, it could result in a smaller required column, and would therefore use less utilities to run.

The final main recommendation of the team is to research the reaction method as well as the catalyst used in this process. As stated previously, there are many different types of catalysts used in industry today to produce acetic acid. The catalyst recommended in this situation is the iridium catalyst. Though this is more expensive up front, it can sufficiently reduce the side products (CO and CO₂), which would reduce the costs of separating the components from the main products as well as scrubbing the toxic gas. The reaction mechanism is also recommended to be researched further. In industry today, the carbonylation of methanol is used as the primary conversion to acetic acid. This could benefit the process if the cost of methanol is less than ethanol, and if the selectivity is higher.

From these recommendations, the team suggests that though the process design meets all product and safe operating parameter requirements, the proposed design is not used until further research is done on eliminating the excess costs.

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