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Comparative Analysis of the Results from the Ideal Gas Assumptions with more Rigorous Calculations from Pro/II of the Production of Pharmaceutical Grade Acetone

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By

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Dedication

To the Almighty God for being my rock and shield

through each moment of my life.

To the best family members, I could ever ask for.

Thank you for your constant prayers, encouragement and support.

To my incredible friends,

Thank you for being a great support system and

For sticking with me.

Acknowledgments

Thank you to Dr. Alex Lopez for your patient and constant assistance in ensuring I understand various chemical engineering materials. Thank you for guidance in making this thesis a success.

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ABSTRACT

The Chemical engineering team was assigned by Landshark Inc to investigate the production of 30,000 tonnes/yr of pharmaceutical-grade acetone with a purity of 99.9 wt.% from the dehydrogenation of isopropanol (IPA). The team was tasked with determining the necessary process and unit operation criteria to ensure the economic feasibility of the proposed plant.

The major goal of this thesis is to provide a data comparison of the reactor in acetone production process when designed in Microsoft Excel and Pro/II. The first part of this thesis will introduce the base case briefly, transition into engineering optimizations and show the results found from the design process as well as some safety concerns to consider when designing these processes.

The purpose of this study was to divulge in greater detail the implications of assuming ideal gas conditions for the process as compared to a more rigorous equations of state. For this study, the reactor section of the plant was analyzed in detail using Microsoft Excel for the ideal gas assumption and Pro//II for more rigorous calculations. The results of this comparative study indicated that Pro//II produced a higher conversion of IPA of 92.3%. This study also showed that results from Pro//II increased profitability and efficiency while decreasing capital and operating costs.

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CHAPTER I

PROCESS DESIGN, PLANT DESIGN & OPTIMIZATION

The sole aim of process design for Chemical Engineers is to generate a product for commercial use. The word “product” encompasses the invention of the new products and how to suit its needs such as temperature conditions, strength, resistance, etc. During this design process stage, various criteria are considered to modify the chemical product and the equipment used in the manufacturing process. This intricate stage, known as the research and development stage involves knowing the desirable properties needed in the input, output and manufacturing process of the design stage.

During plant design, the major question one should ask is “How to design a plant or size equipment around a desired process?” In this project, the goal is to design a reactor around an acetone production process and analyze the results based on the thermodynamic assumptions made. Thermodynamic analysis is important because it helps to understand the overall performance of a system as well as the economic modifications to be made to capital and equipment costs. Simulation software is used to evaluate the thermodynamic assumptions made. For this project, the focus will highlight the ideal-gas law and how it is utilized in Microsoft Excel for analysis. The ideal gas law is a good approximation of the behavior of many gases under certain operating conditions such as higher temperatures and low pressure due to the perfectly elastic collisions from kinetic energy. The low pressure of a system allows for less intermolecular forces among the gas particles. The high temperature systems allow for the gas particles to move quickly within the system while exhibiting low intermolecular collisions with each other. This is due to the energy of the molecules being higher than the intermolecular forces

among the particles. Microsoft Excel is a software that allows for estimations on equations of state, that is why it is more convenient to use ideal gas assumptions for estimated calculations. The base case process is designed in Microsoft Excel because it gives a rough estimate of what the project and real-life scenario of the simulation result would be like. So, the conversion rate, yield and selectivity calculated enables the user to match up what the results would be like with other simulation tools like Pro//II and SimCentral that are widely used in the industries. Other simulations tools mentioned earlier like Pro//II have a variety of lists from which one can choose any equation of state that best suits the design process and which would also match the reactive model.

When analyzing the reactor in this plant design process, two major criteria should be evaluated which are:

1. Equipment-Independent Relationships – These relationships are independent of equipment specifications. Examples are mass balances, energy balances and kinetics.
2. Equipment-Dependent Relationships – These relationships involve equipment specifications. Examples are reactor conversion; pressure drop and residence time.

In a reactor, the kinetics of the reaction is equipment independent in the process. To produce acetone, there is a reversible reaction of the disappearance of IPA which is expressed as the difference between the forward and reverse reaction.

$$(CH_3)_2CHOH \overset{12}{\rightleftarrows} (CH_3)_2CO + H_2 \qquad (1)$$

IPA acetone hydrogen

$$-r_{IPA} = r_1 - r_2$$

$$r_1 = k_1 e^{\frac{-E_1}{RT}} C_{IPA}$$

$$r_2 = k_2 e^{\frac{-E_2}{RT}} C_{Acetone} C_{Hydrogen}$$

$$-r_{IPA} = k_1 e^{\frac{-E_1}{RT}} C_{IPA} - k_2 e^{\frac{-E_2}{RT}} C_{Acetone} C_{Hydrogen}$$

Factors such as concentration, temperature, pressure and catalyst can affect the rate of reaction.

For the equipment dependent relationship, the design equation is dependent on the type of reactor that is utilized in the process. In this process, a Plug-Flow Reactor is modeled in the reaction system for the acetone process. In this system, perfect mixing is assumed in the radial direction at steady-state conditions but not in the axial direction (element upstream or downstream). Ideal gas behavior is adopted with an ideal frictionless flow.

In a PFR, when the reactants go through the pipe, a pressure gradient is required which involves a pressure drop and costs money for pumping. For a small-diameter reactor, pressure drop increases as volumetric flowrate increases. As a result, residence time - the amount of time needed for the reactants to be in the reaction volume reduces. So, with a decrease in residence time, the conversion also decreases because fewer reactants are reacted during a shorter period. Since heat transfer is more efficient for small-diameter reactors because the surface area per volume is larger, the change in temperature in the endothermic reaction decreases causing a lower conversion rate. The reverse will be the case for a large-diameter reactor.

Essentially the primary aim of a chemical process engineer is to produce a product with the least amount of cost needed with all desirable needs ensuring that it is done in the most environmentally safe conditions as well as abiding by the laws of the society and organization.

During process design, the manufactured product is constantly reviewed to understand how to make the process and product better. The optimization process is necessary to reduce

waste, reduce heat and energy sources, reduce raw materials cost while increasing efficiency, improving safety and providing overall profit for the process.

Optimization has to do with selecting the best among various data sets using efficient quantitative methods. The goal of optimization is to find the variables and decision-making approaches in the design process that yield the best value of the performance criterion.

For optimization during design processes, the system must possess certain elements and they are:

- Objective function: this is the measured value of goodness of the optimization problem. The objective function can be cost, profit, yield that needs to be maximized or minimized.
- Predictive model: this model describes the behavior of the system.
- Decision variable: the quantity that appears in the predictive model and depends on the degrees of freedom of a process. These are categorized either as continuous or discrete.
- Constraints: these are limitations on the values of decision variables. These may be linear or nonlinear, and they may involve more than one decision variable.
- The objective function would be to maximize the conversion
- Predictive model: Here, understanding the operating conditions at which the reactor and plant works will enable you to pick the right system for the acetone model. Using the Thermo Package, the Universal-Quasi Chemical (UNIQUAC) is chosen to give the best fit of data.
- The design variable is the inlet high-temperature catalyst which operates between 300°C to 700°C.

There are two types of optimization processes utilized during the design process.

1. Topological optimization
2. Parametric optimization

Topological optimization deals with the topology and arrangement of the process equipment in the plant. Hence, topological optimization should be considered first since it considers the overall profitability of the design plant. Also, when the topological environment is in order, it is easier to interpret the parametric optimization process. So, parametric optimization deals with the design variables such as temperature, pressure, concentration of the design process.

When considering the topological side of optimization, it is important to ask some major questions such as:

1. Can unwanted by-products be eliminated?

   To achieve this, the selectivity of the reactants in the reactor should be maximized. The selectivity of the process which is the rate of desired products to that of the undesired products in the system should be considered. It is beneficial to the process engineers to have a high conversion as well as a high selectivity. Sometimes, this does not happen so keeping that in mind and removing any hazardous by-products to increase the selectivity and maximize conversion is paramount.
2. Can equipment be eliminated or rearranged?

   When changes are made to the base case and optimization process begins, some of the equipment is replaced while some are introduced. It is important to keep this in mind while improving the process.

3. Can alternative separation methods or reactor configurations be employed?

Looking at various alternatives in the distillation column or reactor by changing the pressure, temperature conditions or even the flowrate should be considered to either achieve maximum conversion or achieve much better separation.

4. To what extent can heat integration be improved

   Considering using process streams and less utility streams can further improve the heat integration process and maximize overall profit.

Both topological and parametric optimizations must be performed together with topological optimization at the forefront to make optimization easier and more efficient. In this process, the reactor R-1101 operates at 250°C. When using the high-temperature catalyst, the reactor must operate at a temperature above the standard temperature since the high-temperature catalyst operates within the range of 300°C - 700°C. So, the reactor is set to operate at a temperature gradient of 234°C to 350°C. Nevertheless, this is not feasible since the minimum temperature for the high-temperature catalyst is 300°C. High-pressure steam heated the inlet stream into the reactor; therefore, the reactor inlet could not be heated to 300°C since high-pressure steam allows for the inlet to only get to 244°C. So, by integrating the heating loop into a new heat exchanger (E-1109), 300°C can be generated into the reactor thereby changing the topology of the system. With the new arrangement in the reaction section, the inlet temperature into the reactor is 300°C causing a parametric optimization.

TOOLS UTILIZED DURING PROCESS DESIGN & OPTIMIZATION

Process simulation is used widely in companies and industries and very much by process engineers. It is an important stage that adds value to a predictive model as it progresses from the conception stage through the operational stage. Process simulation and optimization help improve processes for system performance, reliability, productivity and even economical cost. Process simulation is key to identifying parts of design plants that need improvement and optimization.

Chemical engineers implore various tools and software to enable them to design and troubleshoot production processes. Most of the simulation systems adopt a process where they assemble the equations and variables that correspond to the predictive model to solve them simultaneously. A few of these simulation tools that were utilized during this project are Microsoft Excel, Pro//II and SimCentral.

Microsoft Excel is very useful for flowsheet material and mass and energy balance calculations. It is a very appealing software as data can be updated easily just by changing the data and figures. This helps engineers to understand the sensitivity of result changes. Nevertheless, as more data is added and implemented, the spreadsheet becomes very large and unable to navigate through easily and concisely. With Microsoft Excel, you can perform a sensitivity table on your design base case and optimized process. The sensitivity analysis table helps process engineers with decision making as it shows a rough prediction of what a process should be like before and after simulation. In the acetone design process, the sales price and raw materials are the design constraints while labor, utilities and equipment cost are the design variables because they do not have a great impact on the NPV, so their change is insignificant. With these predictions made, the sensitivity analysis on the base case process should be very

similar to that of the optimized case since the sensitivity table helps in indicating the output sensitivity and design model uncertainty.

Solver is also another great tool in Microsoft Excel that highlights your design model decision variables, objective and constraints directly on the spreadsheet. For the design process, Solver takes multiple equations and constraints from the mass and energy balance equations and vapor-liquid equilibrium equations and finds the best solution for the main objective. In correcting the calculations after adding the recycle stream, Solver was run with the objective cell being the flowrate in the recycle stream, and other mass and energy balances, as the solver constraints, while changing their corresponding variables. When all these parameters were input, Solver calculated an approximate new recycle stream because initially the values inputted were guesses which corrected the initial mass balance calculations.

On the other hand, Pro//II is used extensively by chemical engineers to simulate steady-state processes and perform operational analysis. Pro//II provides a wide range of thermodynamic models and data from a large chemical component library that can be explored from. Notwithstanding, Pro//II is very tricky as it involves a lot of troubleshooting to solve complex design operations and to increase overall profit. Pro/II is a very intuitive tool that enables one to know if all the inputted data satisfies the system or if one is missing any information when the system is run. If all information is complete, the interface turns blue as shown in **Figure 1**. If there is missing information, the system will not run but turn red and will turn yellow if most of the information is complete but still needs some update.

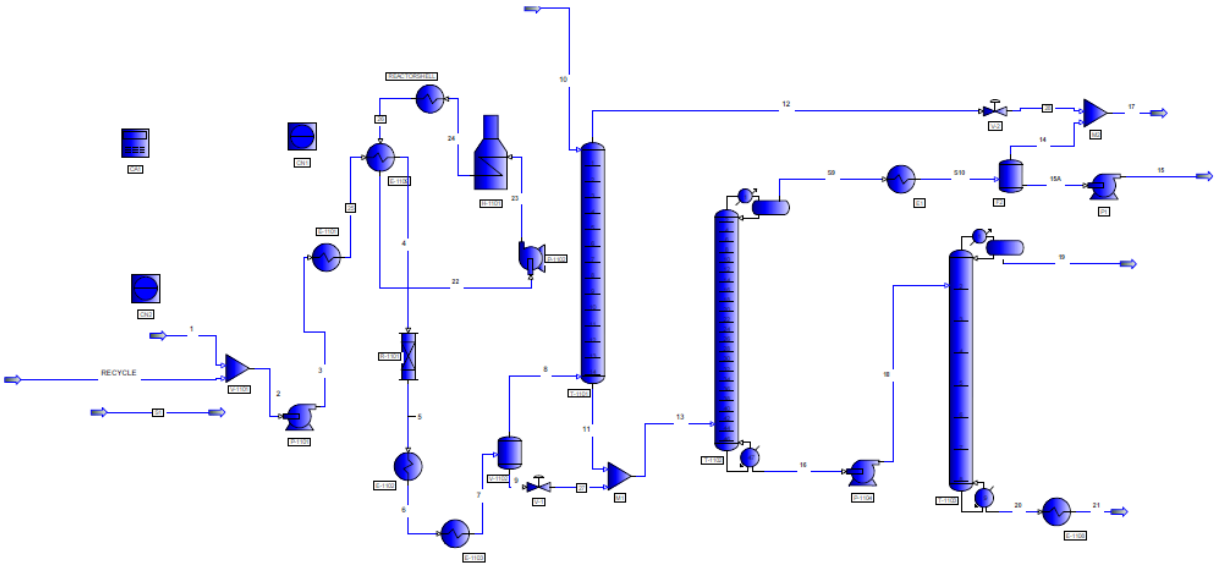

Figure 1: Complete run Pro//II Worksheet indicated with blue color

Pro//II is very easy to navigate and troubleshoot with some basic steps:

1. Build the Process Flow Diagram (PFD) - This is the foundation of the simulation process. Here, you construct the chemical process within the simulation. A modified form of a PFD is constructed. The PFD consists of the process unit operations where material and energy balance information is input as well as the layout of process and utility streams. The PFD of the acetone production is shown below in **Figure 2**.

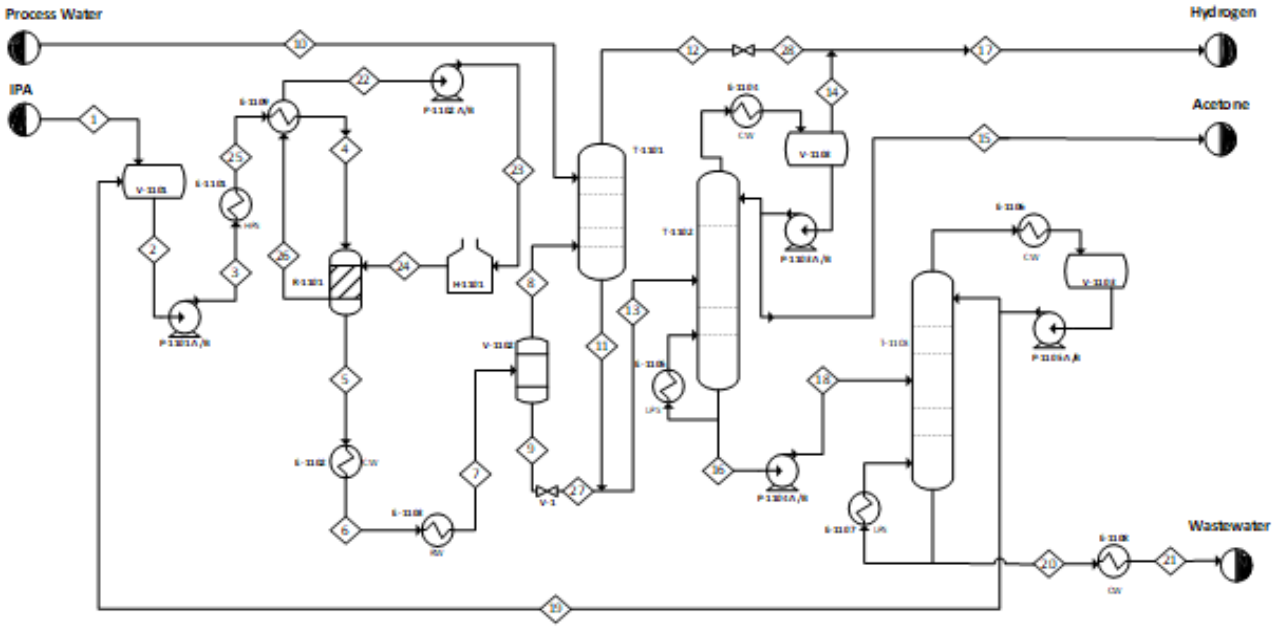

Figure 2: Process Flow Diagram (PFD) of acetone production

During the base case process, various calculations such as mass and energy balances, as well as sizing of each equipment were performed to see if the proposed plant project was economically feasible. The Process Flow Diagram (PFD) is necessary for the information needed during the design process. It is essential that the PFD is easy to follow and interpret and any improvements to the process technology and performance are made during the optimization stage.

For the PFD, there are three basic information needed for the process to work:

1. Process topology
2. Stream information
3. Equipment information

When this basic information on the PFD is missing or has issues, concerns arise and the Process Condition Matrix (PCM) is used to address these issues. PCM is used to analyze and justify

special concerns found in the PFD. For the acetone process, the PCM showed there were areas of special concern for the base case process that warranted further investigation. Guidelines were used from Table 6.1 – 6.4 in *Turton* to determine if the various equipment was operating outside standard conditions.

After the base case process was completed, the optimization of the process began using a design onion model. Through optimization, the Net Present Value (NPV) of the project increased such that the plant demonstrated potential profitability with a positive NPV.

2. Check the Inputs of Measure – This is where you change the units of measure for most quantities to be used in the process. For example, the global default is the English unit of measure
3. Define the Components – This is where you choose the chemical components used in your process form the library
4. Select the Thermodynamic Method – there are various thermodynamic systems listed in this section. The thermodynamic method selected should be based on the physical properties of the chemical components and the operating conditions of the system to get the accurate and best results
5. Supply Process Stream Data – Here, all information concerning feed conditions, flowrates and compositions are entered before the system is run
6. Run the System – when all the necessary and complete information has been fed into the system, you troubleshoot the process by clicking on “Run” in the task bar of the system.

CHAPTER II

SIMULATION PROCESSES

Process simulation is the representation of a chemical process by a mathematical model which is then solved to obtain information about the chemical process. It is the basis for analysis, prediction and testing of mostly a real-life scenario. Process simulation can be seen in various parts of chemical engineering and is made up of:

1. Process Design: the objective of process design is to find the best flowsheet accompanied with mass and energy balance. Some of the flowsheets used for engineering problems are PFDs and Block Flow Diagrams (BFD's).
2. Research and Development: this is where the use of different mathematical models is used and implemented during the design process.
3. Production Planning: this is where the profit of a design process is explored alongside the results gotten from the research stage.
4. Dynamic Simulation: this involves analyzing the various optimal conditions while considering necessary variables and constraints.
5. Training and Education: this involves training operators in charge of the simulation and the processes taken during the startup process of the design plant
6. Optimization: A strategic approach is taken to make the design process better, more efficient and above all cost-effective thereby maximizing profit.
7. Decision making: entails making the best decisions based on the design model, assumptions, calculations and processes used.

All these processes are the building blocks that make simulation possible. Various physical property simulations are used to determine the integrity of an engineering computation. It is essential to understand and know the different computational methods and when best to use a chosen method. Some of the computational methods are UNIQUAC, UNIFAC, Peng-Robinson, NRTL, Soave-Redlich-Kwong, BWRS, Grayson-Streed and Braun-K10. The choice of computational method for simulation is based on four major factors which are:

- The nature of the properties of interest
- The composition of the mixture
- The thermodynamic properties such as temperature and pressure
- The availability of parameters chosen from the Thermopackage shown in **Figure 3**

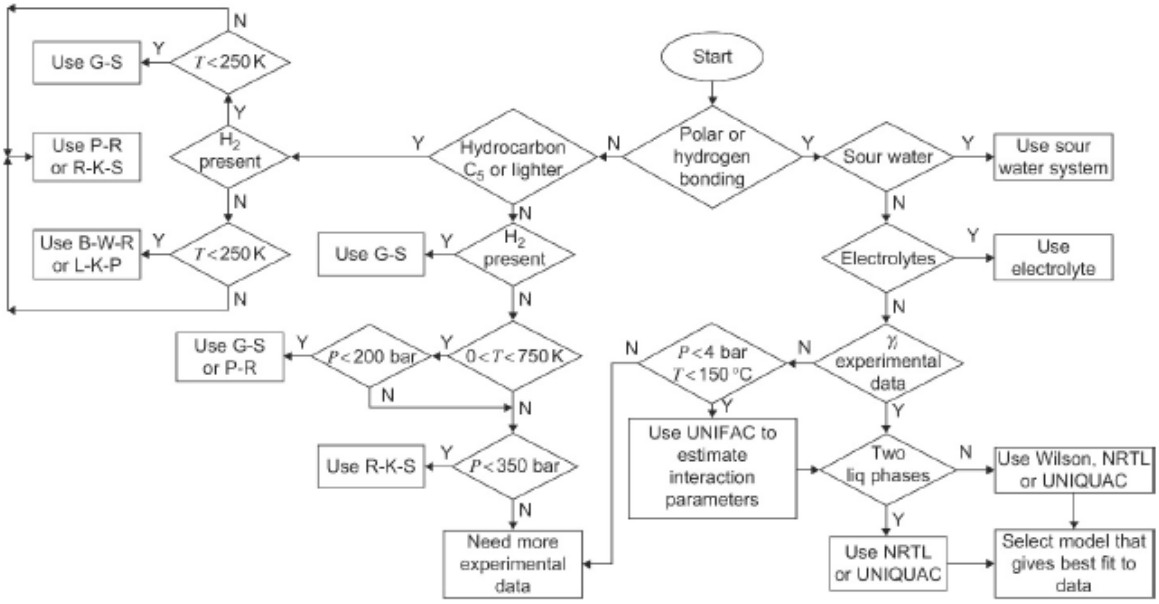

Figure 3: Thermodynamic Package decision tree

THE REACTOR SECTION

According to the design onion hierarchical approach, process design begins at the reactor section and proceeds outward. The reactor design influences every other section of design simulation. The reactor, the heart of the process is the most likely place where the raw materials are converted into products sometimes with the help of a catalyst, so it is essential to start from the reactor if the design process has one. Various design processes and operations based on the thermodynamics, kinetics, transport phenomena coupled with the economic considerations are needed to achieve the utmost desired product. There are various types of reactors used in the industry and the major ones are Plug flow reactor (PFRs), Continuous stirred-tank Reactor (CSTRs), Fluidized Bed Reactors, Membrane Reactors and Tubular Reactors. Different tools are used to model reactive processes of the reactor section. The tools that will be focused on are Microsoft Excel (MS Excel) and Pro/II.

After deeming the base case attractive in the acetone process, the project process was deemed attractive. As a result, various operating conditions such as temperature, pressure, feed conditions are evaluated to be optimized to maximize the Net Present Value (NPV).

As mentioned earlier, the reactor section of the process is evaluated first to improve the NPV. This process started by choosing which catalyst, the high temperature or low temperature, to use in the reactor. To determine the catalyst that results in the greatest NPV, a comparison between the optimum NPVs of the high and low catalyst were analyzed. Also, based on the type of catalyst chosen for the reactor, operating the reactor isothermally, adiabatically or using a temperature gradient had to be selected.

RESULTS

Table 1: High Temperature Catalyst versus Low Temperature Catalyst NPV Breakdown

	HTC ($M)	LTC ($M)
Revenue	467.2	467.2
Materials	(211.6)	(207.5)
Catalyst	(14.3)	(35.4)
Labor	(30.5)	(30.5)
Utilities	(7.9)	(7.5)
Waste Treatment	(0.0)	(0.0)
Income Taxes	(51.8)	(49.1)
Land	(0.9)	(0.9)
Buildings	(2.8)	(2.8)
Machines	(17.1)	(9.2)
NPV	130.3	124.3

The table above shows a breakdown of the cash inflow and outflow of the high-temperature catalyst reactor compared to the low-temperature catalyst reactor.

The cost of materials, catalyst, and machines displayed the largest difference between the optimized high and low-temperature catalyst options. The difference in materials showed that the overall conversion of the high-temperature catalyst must be lower than that of the low-temperature catalyst since it required $4.1 M more raw materials across the span of the project. The difference in the catalyst cost was the determining factor between using the high-temperature catalyst versus the low-temperature catalyst. Also, the low-temperature catalyst must be purchased every 2 years while the high-temperature catalyst only must be purchased every 3

years. Although the machines costs for the low-temperature catalyst were significantly less due to the exclusion of the heating loop, the cost of the catalyst still overcame the reduced machine cost. Based on this result, the high-temperature catalyst was chosen to proceed with for optimization purposes.

USING MICROSOFT EXCEL AS A TOOL

Microsoft Excel was used majorly to calculate the mass and energy balances needed to complete the stream table, equipment sizing and economic analysis of the base case in preparation for the optimization process.

In Microsoft Excel, the ideal gas law is assumed to show the ideality of the system. The ideal gas law combines Boyle's law and Charles law to model and predict the behavior of real gases. The ideal gas law is used as a reference state for equation-of-state calculations and can be used to model gas mixtures at low pressures and high temperatures. Therefore, data is initially inputted into Microsoft Excel before Pro// because Microsoft Excel acts as the baseline to visualize an estimated data of the design system when entered in Pro//II.

Using ideal gas assumptions, the fugacity of a system approaches zero as the activity coefficient approaches 1 where PV = nRT. In this case, the fugacity of the liquid is equal to the fugacity of the vapor phase at equilibrium ($f_i^L = f_i^V$). So, the molecules in the liquid phase are assumed to be identical in size and randomly distributed with negligible interactions. The ideal gas law has a direct effect on the molar volume of the liquid. The activity coefficient and unity fugacity cause the liquid flowrate to increase so that there is more liquid in the recycle stream thereby leading to a decrease in the residence time. This causes the underestimation and decrease in the conversion.

In Reactor R-1101, the Ergun equation was utilized to calculate the pressure drop through the catalyst packed beds. The Ergun equation was modeled using numerical integration to evaluate the reaction kinetics over a series of about 50 intervals. The temperature was assumed to be linear as it was evaluated at each interval. In the base case, the reactor operated at a temperature gradient of 234°C - 350°C. Using the Ergun equation model, the pressure going into the reactor is 2.04 bar at a constant length of 0.1219m.

The Ergun equation is calculated as shown below:

$$\frac{\Delta P}{L} = \frac{150\mu(1-\dot{\varepsilon})^2 u_0}{\dot{\varepsilon}^3 {d_p}^2} + \frac{1.75(1-\dot{\varepsilon})\,\dot{\rho}{u_0}^2}{\dot{\varepsilon}^3 d_p} \qquad (2)$$

Where ΔP = pressure drop
L = height of the bed
μ = fluid viscosity
$\dot{\varepsilon}$ = void space of the bed
u_0 = fluid superficial velocity
d_p = particle diameter
$\dot{\rho}$ = density of the fluid

Table 2: NPV Breakdown of the Excel Case

	Excel Case ($M)
Revenue	472.5
Materials	(212.1)
Catalyst	(14.3)
Labor	(30.5)
Utilities	(8.3)
Waste Treatment	(0.0)
Income Taxes	(52.9)
Land	(0.9)
Buildings	(2.8)
Machines	(17.6)
NPV	133.0

The cash flow process using Microsoft Excel gives a positive NPV of $133M. The sales revenue which is the cash inflow for the design process contributes the most to this project with about $472.5M. With a focus on the reactor and since the high-temperature catalyst is favored over the low-temperature catalyst after analysis, the amount of catalyst does not affect the overall NPV when compared to the raw materials used for the acetone production to be possible.

The single-pass conversion of the IPA reacted is about 88.6% with temperature and pressure operating conditions of 234°C and 2.14 bar respectively.

USING PRO//II AS A TOOL

Pro/II, like Microsoft Excel that performs rigorous mass and energy balances for a range of chemical processes such as the acetone production.

Pro//II uses cubic equations of state such as UNIQUAC, UNIFAC, Peng-Robinson and many others to explore the non-ideality of the design system. The cubic equation of state is a more rigorous equation of state used to predict the thermodynamic properties of chemical components in the system. In this system, the UNIQUAC equation of state models the Gibbs free energy to calculate the activity coefficients to understand the physical property of components. It is used highly in non-ideal systems which in this case Pro//II models the non-ideality of the acetone process. It is also useful in predicting the phase behavior of hydrocarbon mixtures.

Since Pro//II looks at the non-ideality of the system with the UNIQUAC model, the activity coefficient of the liquid phase is calculated using the binary interaction parameters. UNIQUAC model uses an activity coefficient that does not equal 1. For this non-ideal case, the more-than-unity activity coefficient increases the overall fugacity of the system. This leads to a

lower flowrate of liquid out of the reactor and subsequently into the recycle stream thereby increasing the residence time and increasing the conversion of reactants.

Table 3: NPV Breakdown of the Pro//II Case

	Pro//II Case ($M)
Revenue	467.1
Materials	(203.8)
Catalyst	(4.3)
Labor	(30.5)
Utilities	(8.3)
Waste Treatment	(0.0)
Income Taxes	(57.1)
Land	(0.9)
Buildings	(2.8)
Machines	(14.1)
NPV	145.2

Using Pro//II, the NPV increases by $12.2M to a total of $145.2M. The cost of catalyst to be used in the reactor decreases significantly too and yields a greater profit. The raw materials cost also decreases. Using the Pro//II simulation shows an increase in NPV and overall profit while decreasing both capital and operating costs.

Also, the single-pass conversion calculated from Pro//II is calculated to be 92.3%.

Pro//II is much more rigorous than Microsoft Excel and performs a better integration process on the system, which is accounted for in the calculated NPV, costs and single-pass conversion of IPA.

Stream Name		1	2	3	4	5	6
Phase		Liquid	Liquid	Liquid	Vapor	Vapor	Mixed
Temperature	°C	25.00	33.29	33.34	234.00	350.00	45.00
Pressure	BAR	1.01	1.01	2.30	2.16	2.01	1.87
Total Flowrate	KG-MOL/HR	104.37	121.08	121.08	121.08	191.00	191.00
Fluid Rates	KG-MOL/HR						
HYDROGEN						69.92	69.92
ACETONE			0.07	0.07	0.07	69.98	69.98
IPA		69.93	78.90	78.90	78.90	8.99	8.99
WATER		34.44	42.11	42.11	42.11	42.11	42.11
NC-17							

Stream Name		7	8	9	10	11	12
Phase		Mixed	Vapor	Liquid	Liquid	Liquid	Vapor
Temperature	°C	20.00	20.00	20.00	25.00	26.32	34.74
Pressure	BAR	1.73	1.73	1.73	2.00	1.63	1.50
Total Flowrate	KG-MOL/HR	191.00	78.36	112.63	41.50	43.34	76.52
Fluid Rates	KG-MOL/HR						
HYDROGEN		69.92	69.48	0.44		0.11	69.37
ACETONE		69.98	7.85	62.13		3.47	4.38
IPA		8.99	0.23	8.76		0.23	
WATER		42.11	0.80	41.31	41.50	39.54	2.77
NC-17							

Stream Name		13	14	15	16	17	18
Phase		Mixed	Vapor	Liquid	Liquid	Vapor	Liquid
Temperature	°C	21.39	50.00	50.02	92.07	35.45	92.07
Pressure	BAR	1.63	1.20	1.50	1.40	1.20	1.50
Total Flowrate	KG-MOL/HR	155.98	1.52	64.76	89.69	78.04	89.69
Fluid Rates	KG-MOL/HR						
HYDROGEN		0.55	0.49	0.06		69.86	
ACETONE		65.60	1.03	64.50	0.07	5.41	0.07
IPA		8.98			8.98		8.98
WATER		80.85		0.20	80.64	2.77	80.64
NC-17							

Stream Name		19	20	21	22	23	24
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	°C	84.72	109.27	45.00	360.00	360.03	399.38
Pressure	BAR	1.20	1.40	1.26	30.00	30.50	30.25
Total Flowrate	KG-MOL/HR	16.71	72.98	72.98	150.00	150.00	150.00
Fluid Rates	KG-MOL/HR						
HYDROGEN							
ACETONE		0.07					
IPA		8.97	0.01	0.01			
WATER		7.67	72.98	72.98			
NC-17					150.00	150.00	150.00

Figure 4: Microsoft Excel Stream Table of Acetone Production

Stream Name		1	2	3	4	5	6	7
Phase		Liquid	Liquid	Liquid	Vapor	Vapor	Mixed	Mixed
Temperature	°C	25.00	31.35	31.41	300.00	375.00	45.00	20.00
Pressure	BAR	1.01	1.01	2.44	2.16	2.11	1.97	1.83
Total Flowrate	KG-MOL/HR	100.29	113.09	113.09	113.09	180.28	180.28	180.28
Fluid Rates	KG-MOL/HR							
HYDROGEN						67.19	67.19	67.19
ACETONE			0.07	0.07	0.07	67.25	67.25	67.25
IPA		67.19	72.80	72.80	72.80	5.61	5.61	5.61
WATER		33.09	40.23	40.23	40.23	40.23	40.23	40.23
NC-17								
Stream Name		8	9	10	11	12	13	14
Phase		Vapor	Liquid	Liquid	Liquid	Vapor	Mixed	Vapor
Temperature	°C	20.00	20.00	25.00	34.65	29.96	27.97	50.00
Pressure	BAR	1.83	1.83	2.00	1.59	1.50	1.59	1.20
Total Flowrate	KG-MOL/HR	74.95	105.34	171.50	177.07	69.37	282.41	2.39
Fluid Rates	KG-MOL/HR							
HYDROGEN		66.75	0.44		0.39	66.36	0.82	0.76
ACETONE		7.32	59.94		6.25	1.07	66.19	1.62
IPA		0.14	5.47		0.14		5.61	
WATER		0.74	39.49	171.50	170.29	1.94	209.78	
NC-17								

Stream Name		15	16	17	18	19	20	21
Phase		Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid
Temperature	°C	50.02	101.77	31.68	101.77	84.96	105.98	45.00
Pressure	BAR	1.50	1.52	1.20	1.60	1.20	1.25	1.11
Total Flowrate	KG-MOL/HR	64.77	215.25	71.76	215.25	12.81	202.45	202.45
Fluid Rates	KG-MOL/HR							
HYDROGEN		0.06		67.13				
ACETONE		64.50	0.07	2.69	0.07	0.07		
IPA			5.61		5.61	5.61	0.01	0.01
WATER		0.21	209.57	1.95	209.57	7.13	202.44	202.44
NC-17			0.00					
Stream Name		22	23	24	25	26	27	28
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Mixed	Vapor
Temperature	°C	400.00	400.05	437.35	244.00	406.65	19.97	29.96
Pressure	BAR	29.75	30.50	30.25	2.30	30.00	1.59	1.20
Total Flowrate	KG-MOL/HR	150.00	150.00	150.00	113.09	150.00	105.34	69.37
Fluid Rates	KG-MOL/HR							
HYDROGEN							0.44	66.36
ACETONE					0.07		59.94	1.07
IPA					72.80		5.47	
WATER					40.23		39.49	1.94
NC-17		150.00	150.00	150.00		150.00		

Figure 5: Pro//II Stream Table of Acetone Production

Table 4: Utility Summary

Utility Summary									
Equip Tag No	**E-1101**	**E-1102**	**E-1103**	**E-1104**	**E-1105**	**E-1106**	**E-1107**	**E-1108**	**E-1109**
Utility	hps→bfw	cw→cw ret	rw→rw ret	cw→cw ret	lps→bfw	cw→cw ret	lps →bf w	cw→c w ret	NC 17→N C 17
Duty (GJ/h)	5.5	4.03	0.93	11.01	14.49	1.82	1.86	0.93	0.77

Table 5: Reactor Summary

Reactor	
Tag No	**R-1101**
Type	Fixed TS
Area (m2)	132.9
Shell side	
MOC	CS
Phase	Liquid NC17
Tube side	
MOC	CS
Phase	Vapor
Catalyst Volume (m3)	1.7

CHAPTER III

CONCLUSION

The major goal of this study is to analyze the differences between the ideal gas assumptions and thermodynamics associated with Microsoft Excel and Pro//II. The results of the comparative study indicate that Pro//II provides a better estimate when calculations of the predictive model are calculated over Microsoft Excel. With Microsoft Excel, the ideal gas law is assumed so the calculations and data derived are a rough prediction of what the design model will look like. Whereas, simulation tools like Pro//II give results based on the non-ideality of the system hence, taking a more equation of state into account. The non-ideality nature of the system allows for a more accurate result when Pro//II is used.

In Excel, estimates that are mathematically possible but not feasible in real life are permissible because Excel runs only numbers without taking into consideration the practicality of decisions made. On the other hand, simulating in PRO/II will show the errors in judgment made when deciding optimum values to use for the variables. For example, if an inlet pressure specified into a distillation column is lower than the outlet pressures in the condenser and reboiler, Excel will give mathematical numbers for whatever optimum choice is made, while PRO/II will give an error in results, stating that the assumptions are not achievable in real-life scenarios.

Another difference in both simulations is that the approximations made by excel are done using linear equation - ideal gas law, while the approximations made by PRO/II are done using the exponential cubic equation of state - UNIQUAC series of equations. The assumption of the

ideal gas system accounts for the fugacity to be lower when compared to the non-ideal gas system. The lower fugacity accounts for the underestimation of the conversion on IPA in the process. For the non-ideal case, UNIQUAC uses activity coefficients to predict an increase in the overall fugacity of the system. Hence, the Pro//II system gives a higher conversion than the ideal gas case.

PROCESS SAFETY AND ENVIRONMENTAL CONCERNS

The implementation of process safety began at the start of the optimization process to prevent hazards and accidents within the acetone facility. There are key concerns to be taken into consideration regarding safety.

The Safety Data Sheets (SDS) should be utilized to enable operators and engineers to understand the major differences between the physical and chemical properties of the chemical substances used in the chemical plant.

All personnel should always be equipped with Personal Protective Equipment (PPE) when in the acetone plant. Each employee must wear flame-retardant full body suits as well as gloves with the ability to withstand the corrosivity of acetone. Hard hats and high chemical resistant rubber, steel-toed boots should be worn to further prevent injury. Vapor monitors attached to either the hard hats or full-body suits must always be worn to ensure breathable air quality.

Regrading process safety, control systems should be implemented to ensure the process runs at the specified conditions and making sure that the materials of the equipment can withstand the process conditions. Regular check-ups on the equipment should be made as specified by the equipment manufacturers.

For the raw materials and chemical components involved in the design process, it is important to understand their physical and chemical properties to be able to protect yourself from any potential hazardous substances.

IPA is a very flammable chemical whether in vapor or liquid form. It is also a colorless chemical with an alcohol-like odor. It is important to have adequate ventilation and explosion-

proof equipment. Engineering controls should be adopted to keep dust or vapor concentrations below lower explosive limits. During and after process operation, it is necessary to eliminate any ignition sources that can ignite with the chemical to cause fire.

Hydrogen, a by-product of the acetone process is explosive so eliminating sources of ignition such as sparks from electrical equipment, static electrical sparks or open flames should be adhered to strictly. Hydrogen is also prone to leakage and very difficult to detect due to its odorless nature. Careful evaluation and purge operations should be used to prevent the formation of flammable or explosive mixtures. It is also important to have good ventilation to reduce the formation of flammable mixtures and prevent any potential hazard of asphyxiation.

NC-17 is toxic if ingested. Acetone is highly flammable, can cause serious irritation to the eyes and skin, and can also cause dizziness. It is important to store it in a cool and well-ventilated place free from heat and ignition sources. All storage of chemicals should align with the Occupational Safety and Health Administration's standards.

Acetone evaporates rapidly and when it is in the atmosphere, it is degraded by UV light with a 22-day half-life. Acetone also dissipates slowly in soil, animals, or waterways since it is sometimes consumed by microorganisms and can move into groundwater from spills or landfills. Acetone may pose a significant risk of oxygen depletion in aquatic systems due to the consumption by microbial activity. Ensure that run-off acetone is disposed of properly to avoid inhalation and evaporation of a large amount of acetone into the atmosphere. The wastewater stream should be treated to have below 0.1 wt.% organics before it is sent to the wastewater treatment facility. Before leaving the wastewater treatment facility, it must meet the Environmental Protection Agency's (EPA) standards.

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