ANNUAL PRODUCTION OF 400,000 TONNES OF PURE TEREPHTHALIC ACID FROM CRUDE TEREPHTHALIC ACID VIA CRYSTALLIZATION

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CERTIFICATE

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ABSTRACT

The report designs and operates a Purified Terephthalic Acid (PTA) plant that will run parallel with an existing plant to increase production capacity and eliminate bottlenecks. The study begins by emphasizing PTA production and the problem. A comprehensive literature review covers PTA basics, methods for converting Crude Terephthalic Acid (CTA) to PTA, and PTA crystallization processes. This literature evaluation lays the groundwork for the planned study and future research. It then presents a process flow diagram and details of PTA production procedures. CTA, Hydrogen, Water/Steam and Nitrogen are important raw materials for production of high-quality PTA. Design criteria for equipments such as Feed tank, Pumps, Pre-heaters, Reactor, Crystallizers, Centrifuges, and Dryers will be carefully studied. Material and energy balances were carefully examined across these equipments. Thesis also covers critical equipment component design and specifications. The design, function, and design considerations of shell-and-tube heat exchangers are examined. Includes packed-bed reactor design and reactions. The crystallizer's design and operation are analyzed. Aspen Hysys and Aspen Plus software simulate process dynamics and behavior, providing a complete picture. Component lists, fluid packages, parameters, and reactor and crystallizer requirements are simulated. Simulations reveal process performance and enable optimization. This thesis assesses primary equipment costs, total investment, direct production expenses, income generation, and payback period for any industrial operation. These financial studies reveal the parallel PTA plant's economic viability. Hazard and Operability (HAZOP) research identifies process hazards and recommends risk assessment and reduction. Explaining HAZOP and identifying process hazards ensures safety and regulatory compliance. This final-year thesis suggests designing and operating a PTA factory alongside an existing facility to boost production capacity and eliminate bottlenecks. Process overview, material and energy balance calculations, equipment design, simulation, instrumentation and control strategies, cost estimation, and HAZOP studies are examined in detail to inform future research.

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CHAPTER 1

INTRODUCTION

1.1 Project Description

This section gives a general description of the project emphasizing the crystallization-based purification of terephthalic acid (PTA). By creating a PTA facility that can run in parallel with an existing plant and accommodate an additional 1095 tons of feed per day, the project seeks to alleviate a production bottleneck.

Industrial Application of Terephthalic Acid: The manufacturing of polyethylene terephthalate (PET), a widely used polymer with multiple industrial applications, requires terephthalic acid as a crucial raw material. The production of bottles, fibers, films, and other packaging products uses PET predominantly. It is widely used in the beverage sector to make bottles for soft drinks and water, and in the textile industry to make polyester fabrics and fibers. Various household and personal care items, including food containers, cosmetics, and detergents, are also made from PET.

A typical purification process is given below:

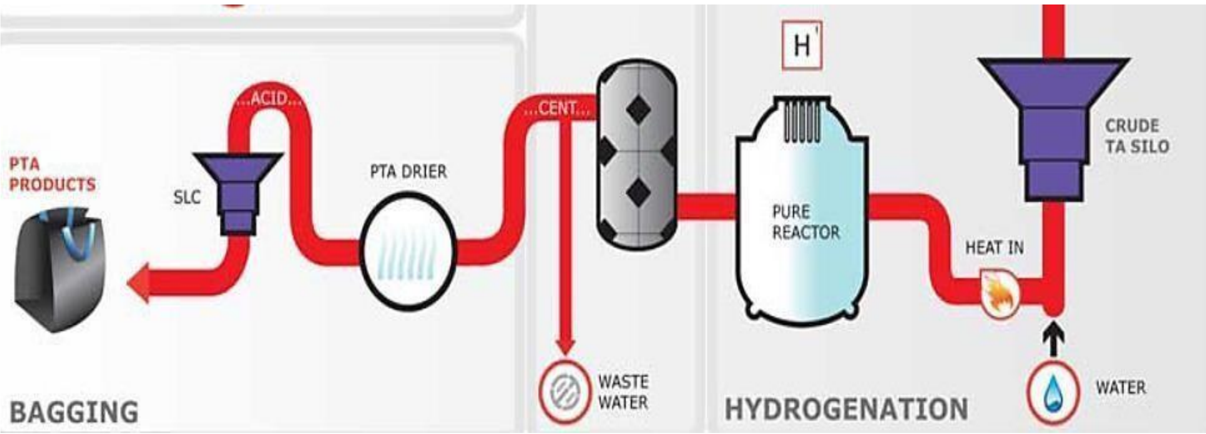


Figure 1 General CTA Purification Process

1.2 Importance of Improving PTA Production Purity

This thesis's problem statement centers on the requirement to raise PTA's purity from 99.7% to 99.98%. The performance and characteristics of PET-based goods can be significantly impacted by even a small increase in purity. PET is suitable for demanding applications because higher purity PTA offers increased mechanical strength, thermal stability, and chemical resistance. Higher purity levels are also necessary to meet the exact quality standards demanded by sectors like food and beverage packaging. Moreover, the presence of 4-CBA acts as a terminating agent in the polymerization of PET and hence needs to be removed.

The primary goal of this final-year thesis is to create a PTA plant that runs concurrently with the current plant and has the capacity to accept an extra 1095 tons of feed per day. The project's goal is to boost overall PTA production capacity and satisfy the expanding market demand for high-quality PTA by tackling the production bottleneck that is currently hindering progress. To achieve the requisite purity level of 99.98%, the thesis focuses on streamlining the crystallization process used to convert CTA to PTA.

The PTA industry has grown significantly during the past few years. This increase might be ascribed to the rising packaging and consumer products sectors, notably in places like Asia-Pacific. PTA is a primary constituent in many PET-based products, which are in high demand due to reasons like population expansion, urbanization, and shifting consumer lifestyles. It is crucial to streamline the PTA production process and deal with any bottlenecks preventing increasing production to satisfy the growing demand.

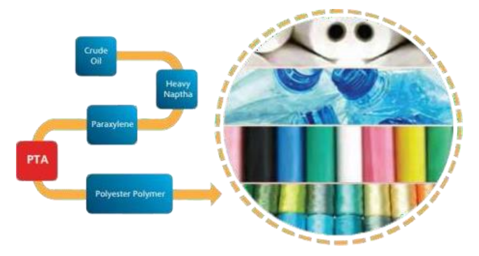


Figure 2: PTA Applications Downstream

CHAPTER 2

LITERATURE OVERVIEW

2.1 Overview of Purified Terephthalic Acid (PTA):

Purified Terephthalic Acid (PTA) is a crucial intermediate in the production of polyethylene terephthalate (PET), a widely used polymer with various industrial applications. PTA is obtained through the purification of Crude Terephthalic Acid (CTA), which is derived from the oxidation of para-xylene. PTA possesses superior chemical and physical properties, making it suitable for manufacturing high-quality PET products. The chemical formula of Terephthalic Acid is $C_8H_6O_4$.

PTA serves as a key building block for PET production, contributing to its mechanical strength, thermal stability, and chemical resistance. The quality and purity of PTA significantly impacts the performance and properties of PET-based materials. Achieving a high level of PTA purity, such as 99.98%, ensures the production of PET with enhanced mechanical properties and reduced defects.

2.2 CTA to PTA Conversion Method:

Crude Terephthalic acid is converted Pure Terephthalic acid via Hydrogenation of the impurities present in the crude variant. These impurities include polyaromatic compounds which are responsible for discoloration of the Crude Terephthalic, and their presence is deemed undesirable in the final product. Moreover 4-Carboxybenzaldehyde is a terminating group in the polymerization of PET for which purified terephthalic acid is used as a monomer. Hydrogenation of polyaromatic colored impurities converts them into colorless forms while 4-CBA is converted into para-toluic acid which can be separated via crystallization to yield Purified Terephthalic Acid.

The Reactions for the conversion of the conversion of CTA to PTA is given below:

$$4\text{-}CBA + H_2 \longrightarrow 4\text{-}HMBA + H_2 \longrightarrow p\text{-}TA + H_2O$$

Non-colored impurities or

Colored impurities + Hydrogen ⟶

Soluble colored Impurities

2.3 Crystallization Techniques in PTA Production:

Crystallization plays a vital role in the production of high-purity Terephthalic Acid. Various crystallization techniques have been explored to optimize the process and improve the purity of the final product. These techniques include cooling crystallization, antisolvent crystallization, reactive crystallization and flash crystallization.

2.3.1 Cooling Crystallization:

Crude Terephthalic Acid (CTA) dissolved in a suitable solvent (such as water) is subjected to controlled cooling. As the solution cools, Purified Terephthalic Acid (PTA) crystals start to form, which can be separated from the solvent through filtration or other separation techniques.

2.3.2 Antisolvent Crystallization:

In antisolvent crystallization, CTA is dissolved in a solvent (such as water), and an antisolvent (e.g., a polar organic solvent) is added to the solution. The addition of the antisolvent reduces the solubility of PTA, leading to the precipitation of PTA crystals. The PTA crystals can then be separated from the solvent-antisolvent mixture.

2.3.3 Reactive Crystallization:

Reactive crystallization involves the use of a reactive additive or reactant during the crystallization process. The reactant reacts with CTA to form PTA crystals and generates a byproduct. This process helps in enhancing the purity and yield of the PTA crystals.

2.3.4 Flash Crystallization:

A phenomenon called flash crystallization occurs when a solvent evaporates, rapidly cooling a solution. The solute precipitates out of solution as tiny, homogeneous crystals as a result of the rapid cooling. A variety of crystals, including those for pharmaceuticals, food additives, and industrial chemicals, can be created using the flexible technique of flash crystallization. The required component is first dissolved in a solution before flash crystallization can take place. The liquid is poured into a flash crystallizer, which sprays it into a lower-pressure chamber. The temperature of the solution rapidly decreases as the solvent evaporates. The solute will precipitate out of solution when the solution's temperature hits its saturation point. The temperature of the solution, the solute's concentration, and the size of the droplets are only a few of the variables that affect how quickly crystals form in a flash crystallizer. The solution's temperature needs to be low enough to encourage crystallization while not being too low to cause the solute to crystallize too slowly. The solute concentration must be sufficient to encourage crystallization without growing crystals to unacceptably large sizes. The size of the droplets should be just right to encourage nucleation while preventing them from dissipating too quickly and preventing crystallization.

CHAPTER 3

PROCESS OVERVIEW

3.1 Process Flow Diagram

The PFD, which shows the order of unit operations and the flow of materials, provides a visual picture of the PTA production process. The PFD describes the primary machinery and significant processes in the conversion of CTA to pure terephthalic acid.

The CTA feed enters the system at a specific flow rate to start the PFD. The water serves as the solvent as it is combined with the CTA feed in a feed tank. Centrifugal pumps are then used to transfer the mixture to the pre heaters that then transfer it to the packed bed reactor (PBR), where CTA is transformed into PTA. The creation of PTA crystals occurs in the PBR as a result of the required reactions being facilitated by the palladium-coated carbon catalyst.

Following PBR, the reaction mixture proceeds through flash evaporation in the crystallizers. This lowers the pressure and temperature of the reaction mixture, which encourages the growth of PTA crystals. A centrifuge is then used to separate the PTA crystals from the liquid phase, and the waste filtrate is sent to a recycle tank as mother liquor. To be processed further, the mother liquor is recycled back into the feed tank.

After being extracted from the centrifuge, the PTA crystals are passed to a steam tube rotary drier, where extra moisture is drained away to produce dried PTA crystals. The PTA crystals are recovered after drying and may then be packaged or processed further.

The process flow diagram offers a thorough breakdown of the PTA manufacturing process, enabling a better understanding of the machinery used and the order of steps.

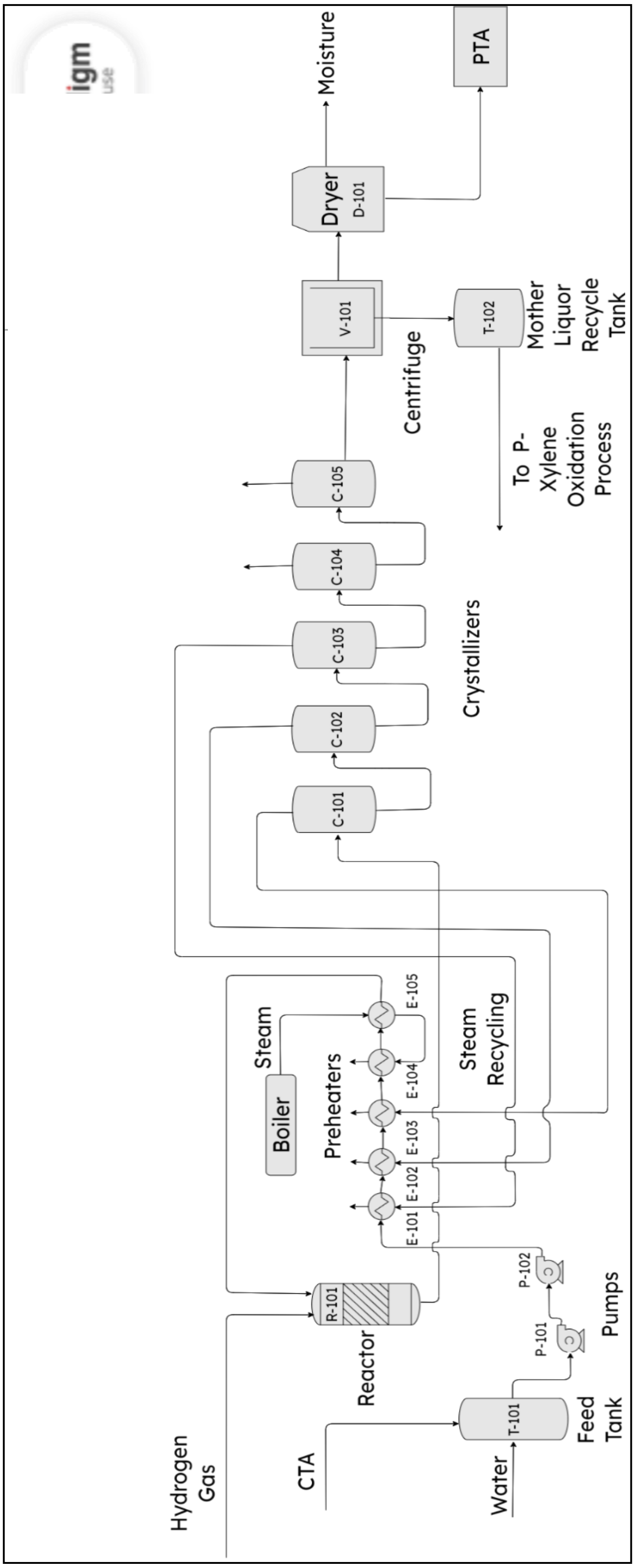


Figure 3: Process Flow Diagram

3.1.1 Process Description

The synthesis of high-quality Purified Terephthalic Acid (PTA), with a target purity of 99.98%, was the goal of the experimental design, which attempted to optimize the crystallization process. The impacts of various process factors on the crystallization process were examined through a series of laboratory-scale studies.

Five crystallizers and a packed bed reactor comprised the experimental setup. Crude terephthalic acid (CTA), which was fed into the process at a rate of 62,586 kg per hour and contained impurities like 4-Carboxybenzaldehyde (4-CBA) at a rate of 167.9 kg per hour, was the initial feed. A water feed rate of 152,982 kg/hr and a hydrogen feed rate of 13.3 kg/hr were added to the CTA feed. Pumps were used to increase the stream pressure to 82barg. The stream was then sent to a series of five heat exchangers to achieve the required 283 degree Celsius temperature. For the intended chemical reactions to occur, the packed bed reactor created the requisite conditions.

The conversion of CTA to PTA and the elimination of impurities were made possible by operating the reactor under a particular temperature and pressure settings. Flash evaporation took place in crystallizers, which resulted in a drop in temperature and pressure. This phenomenon contributed to the development of PTA crystals in a suitable environment.

The stream from the reactor outlet was then routed toward the five crystallizers. To cause PTA to crystallize, the crystallizers used cooling methods such as flash evaporation. The temperature dropped as a result of the flash evaporation, which involved lowering the pressure in the crystallizers. The production of PTA crystals was aided by the drop in temperature while impurities were left behind. The residence duration, temperature, and flash evaporation procedures were all optimized in the design of the crystallizers for quick crystal formation and separation.

The PTA crystals were moved from the crystallizers to a centrifuge for filtration. The mother liquor, which contained undesired contaminants and leftover solvents, was successfully removed from the crystals by the centrifuge. The PTA crystals were separated, and after that they were transferred to a steam tube rotary dryer to finish drying and get rid of any remaining moisture.

The mother liquor, or undesirable filtrate, was simultaneously gathered and sent to a recycle tank. This mother liquor, which contained contaminants that had been dissolved, was recycled back to the feed tank and then put back into the system. This recycling procedure reduced waste and improved workflow.

3.2 Raw Material

3.2.1 Crude Terephthalic Acid (CTA)

With the molecular formula $C_8H_6O_4$, crude terephthalic acid (CTA), also known as CTA, was used as the initial substance for the crystallization procedure. Impurities such 4Carboxybenzaldehyde (4-CBA) and colored impurities, which were known to impair the purity of the final PTA product, were present in the CTA utilized in the experiment. To get the desired level of PTA purity, it was essential to get rid of these contaminants. Terephthalic acid (PTA), a crucial ingredient in the manufacturing of polyester, is produced from crude terephthalic acid (CTA), a byproduct of the process. CTA is typically created by oxidizing p-xylene and includes a variety of impurities, such as:

- 4-carboxybenzaldehyde (4-CBA)
- p-toluic acid (p-TOL)
- Benzoic acid (BZ)
- Colored polyaromatics

Depending on the manufacturing method, the impurity levels in CTA can vary, although they are normally in the range of 2000–5000 ppm for 4-CBA and 100–200 ppm for p-TOL and BZ. Although the colored polyaromatics are frequently found at smaller concentrations, they can give CTA a yellow or brown hue.

The contaminants in CTA may cause a variety of detrimental outcomes, such as:

- Lowering PTA's purity
- Increasing PTA's viscosity
- Resulting in PTA's discoloration
- Lowering the polyester yield

For these reasons, it's crucial to clean the CTA of contaminants before converting it to PTA. The most popular technique for purging contaminants from CTA is hydro purification, which transforms the pollutants into innocuous molecules using a catalyst.

The colorless liquid 4-carboxybenzaldehyde (4-CBA) has a pungent odor. It is a monocarboxylic acid that is created when p-xylene is oxidized. Although 4-CBA is a relatively insignificant contaminant in CTA, it can significantly affect the PTA's color and purity.

The colorless liquid p-toluic acid (p-TOL) has a pungent odor. It is a monocarboxylic acid that is created when toluene is oxidized. Although p-TOL is a relatively insignificant contaminant in CTA, it can significantly affect PTA's color and purity.

White solid benzoic acid (BZ) has a faint odor. It is a monocarboxylic acid that is created when benzene is oxidized. Although BZ is a relatively insignificant contaminant in CTA, it can significantly affect the PTA's color and purity.

A class of chemicals known as colored polyaromatics are created when organic matter burns partially. They usually exist in little amounts in CTA, but they can give it a yellow or brown hue. The yield of polyester might also be adversely affected by colored polyaromatics.

3.2.2 Hydrogen

The hydro purification technique creates PTA from CTA using hydrogen as a basic ingredient. In this procedure, the contaminants in CTA are converted to safe chemicals by passing hydrogen across a catalyst like palladium on carbon. These steps often involve the reduction of 4-carboxybenzaldehyde (4-CBA), p-toluic acid (p-TOL), and benzoic acid (BZ) impurities.

As it eliminates contaminants that could have a detrimental effect on PTA quality, the hydro purification process is a crucial stage in the production of PTA. Because the impurities are changed into chemicals that may be recycled or sold, the hydro purification procedure also boosts the yield of PTA.

It is only recently that hydrogen has been used in the hydro purification procedure. In the past, a procedure known as distillation was used to get rid of the contaminants in CTA. However, distillation consumes a lot of energy and can result in PTA that is tainted with minute amounts of contaminants. The hydro purification procedure creates PTA that is free of contaminants while using less energy.

There are several advantages to using hydrogen in the hydro purification process. First off, compared to distillation, it is a more energy-efficient process. Second, it generates PTA that is impurity-free. Third, since there are no hazardous emissions produced, it is a more environmentally friendly procedure than distillation.

A crucial component in the creation of high-quality PTA is the use of hydrogen in the hydro purification procedure. In comparison to conventional procedures, the hydro purification procedure effectively removes contaminants from CTA while using less energy and harming the environment. As a result, the hydro purification method that uses hydrogen to produce PTA is becoming more widely used.

3.2.3 Water/Steam

When PTA is made from CTA, water is not a raw ingredient. Nevertheless, it serves as a solvent throughout the purifying process. After being crystallized, crude terephthalic acid (CTA) is then dissolved in water. In order to turn contaminants into para-toluic acid, hydrogen is added to the solution, and it is then passed through a hydrogenation reactor.

After being cleaned, PTA is crystallized and dried.
There are various benefits to using water in the purifying process. It is a relatively cheap solvent, to start with. Second, it is safe for the environment and non-toxic. Thirdly, it aids in the removal of

contaminants that are challenging to eliminate through mechanical means, such as 4-carboxybenzaldehyde (4-CBA).

There are certain drawbacks to using water in the purification phase as well. First off, it might raise the price of production. Second, it might make the process use more energy. Third, it can make the equipment more susceptible to rust.

3.2.4 Nitrogen

Nitrogen is applied in a variety of different methods to facilitate the enhancement of the purification process when separating PTA from CTA. In the first place, it is utilized in nitrogen blanketing, which involves the formation of a defensive layer all the way around the PTA distillation column. This serves the purpose of preventing the oxidation of PTA, which can lead to polymerization as well as the generation of byproducts that are not acceptable. Additionally, in the PTA crystallization unit, nitrogen sparging is used to prevent the production of air bubbles within the PTA. This is done by removing excess nitrogen from the PTA. Cloudiness in the PTA can be caused by air bubbles, which can also lead to the production of undesirable byproducts. In addition, nitrogen is used in the process known as nitrogen drying, which removes any trace of moisture that may have been present in the PTA product. PTA is susceptible to breakdown over time when exposed to moisture, which also promotes the production of undesirable byproducts. Because nitrogen is an inert gas, it does not react with other compounds. As a result, it is an excellent candidate for the purification of PTA. In addition, nitrogen is available at a price that is not prohibitively expensive, making it a viable option for use in purifying procedures. Nitrogen's applications in the PTA purification process give many benefits to the process as a whole, including the prevention of oxidation, the prevention of the production of air bubbles, and the effective drying of the PTA product.

3.3 Equipment

3.3.1 Feed Tank

To store, regulate the flow of raw materials, and their mixing, into the process, feed tanks are employed. In this instance, water and crude terephthalic acid (CTA) are stored in feed tanks. The feed tanks make sure that the raw ingredients enter the process in a steady and controlled flow, enabling precise dosing and mixing.

3.3.2 Centrifugal Pumps

Slurry pumps and centrifugal pumps are crucial tools in the process of turning crude terephthalic acid (CTA) into purified terephthalic acid (PTA). Slurry pumps are used to move slurries of CTA and other chemicals throughout the purification process, whereas centrifugal pumps are used to move CTA from storage tanks to the purifying process.

Fluids are moved by centrifugal force in centrifugal pumps. High-speed impeller rotation of the pump causes centrifugal force, which forces the fluid outward. Following that, the fluid exits the discharge outlet after passing through the pump casing. Applications requiring large volume, low pressure often call for centrifugal pumps.

Slurry pumps are a particular kind of centrifugal pump made for handling fluids with solid particles. The solids may be heavier than the fluid or they may be floating in them. Slurry pumps are made to handle higher pressures and often have a larger impeller than centrifugal pumps.

Centrifugal pumps are utilized to move CTA from storage tanks to the purifying process in the manufacturing of PTA. The PTA is created by the reaction of the CTA with oxygen after the CTA has been heated to a high temperature and injected into a reactor.

During the purification procedure, slurries of CTA and other chemicals are moved using slurry pumps. The slurries are treated in a number of tanks and reactors after being pumped there. The high temperatures and pressures of the purifying process must be handled by the slurry pumps.

Slurry pumps and centrifugal pumps are crucial tools in the manufacture of PTA. These pumps are employed throughout the industrial process to move liquids and slurries. High temperatures, high pressures, and caustic chemicals must all be handled by the pumps in order to produce PTA.

- Increased efficiency: Centrifugal pumps and slurry pumps can move fluids and slurries more efficiently than other types of pumps. This can lead to reduced energy costs and improved production rates.
- Improved safety: Centrifugal pumps and slurry pumps are designed to handle hazardous chemicals. This can help to reduce the risk of accidents and injuries.
- Increased reliability: Centrifugal pumps and slurry pumps are built to last. This can help to reduce maintenance costs and improve uptime.

To make it easier to transfer the CTA and water from the feed tanks to the packed bed reactor, two centrifugal pumps are used. Due to their capacity for handling large flow rates and supplying enough pressure to move the fluids through the process, centrifugal pumps are used. They provide dependable and effective functioning, guaranteeing a constant and stable supply of raw resources.

3.3.3 Pre-Heater

Preheaters are used to heat the crude terephthalic acid (CTA) before it enters the hydro purification reactor in the purification of PTA from CTA.

There are numerous various kinds of preheaters, but the shell and tube heat exchangers are the most typical ones used in the manufacturing of PTA. A shell and tube heat exchangers are made up of a number of tubes encased in a shell. The heat source, which is steam from the crystallizers, is cycled through the shell while the CTA is pumped through the tubes.

Preheaters are used in the manufacturing of PTA because they have many advantages. First, preheaters can aid in increasing the industrial process' efficiency. The reaction can happen faster and at a lower temperature by heating the CTA before it enters the hydro purification reactor. The TA is soluble in water at higher temperatures, which speeds up the chemical process. Due to the high temperature and pressure requirements in the industrial facility, shell and tube heat exchangers are used. Five heat exchangers are used in the final design to help with heat transfer and temperature regulation.

3.3.4 Packed Bed Reactor

Chemical reactions that use solid catalysts in tubes or vessels are known as packed bed reactors. The catalyst encourages the chemical interaction between the reactants as they flow through the bed. Packed bed reactors are frequently utilized while converting CTA into PTA.

Terephthalic acid (TA) is initially produced by oxidizing crude terephthalic acid (CTA), which is then used to make PTA. After that, the TA is hydrogenated to create PTA.

A palladium catalyst that is crammed into a packed bed reactor catalyzes the hydrogenation reaction.

High pressure and temperature TA is poured through the bed. The hydrogenation reaction is accelerated by the palladium catalyst, resulting in the conversion of TA to PTA. After cooling, the PTA is collected.

A sort of packed bed reactor called a trickle bed reactor has the catalyst in the form of a solid and the reactants in the form of a liquid or slurry. In order to produce PTA from CTA, trickle bed reactors are frequently employed since they offer a good balance between efficiency and cost. The hydrogenation of TA to PTA, the second phase in the production process, is carried out in trickle bed reactors. The trickling bed reactor offers a good approach to evenly distribute the catalyst throughout the liquid phase of the hydrogenation reaction, which is a liquid-phase reaction.

Benefits of producing PTA in trickle bed reactors include:

- High efficiency: Trickle bed reactors can achieve high conversion rates, which can lead to reduced energy costs and improved production rates.
- Low cost: Trickle bed reactors are relatively inexpensive to construct and operate.
- Versatile: Trickle bed reactors can be used for a variety of reactions, which can make them a valuable asset in a chemical plant.

However, employing trickle bed reactors has significant drawbacks as well:

- Pressure drop: Because of the packed bed's potential to significantly lower pressure, maintaining the appropriate flow rate may involve the usage of pumps.
- Deactivation of the catalyst: As the catalyst ages, the reactor's efficiency may be lowered.
- Clogging: The packed bed may become clogged over time, which may lower the reactor's flow rate and efficiency.

Chemical reactors known as trickling bed reactors are adaptable and effective for a range of processes, including the generation of PTA. The possible downsides of employing trickle bed reactors, such as pressure decrease, catalyst deactivation, and clogging, must be understood, though.

3.3.5 Crystallizer

The process of turning a liquid or supersaturated solution into a solid crystalline form is known as crystallization. Crystallizers are used to create pure crystals for making PTA from CTA.

There are several different kinds of crystallizers, but the flash crystallizer is the one used most frequently in the manufacture of PTA. A flash crystallizer is a particular kind of continuous crystallizer where crystallization is induced by rapidly cooling or concentrating the supersaturated solution.

There are various advantages to using flash crystallizers in the manufacture of PTA. First, PTA crystals with a restricted size distribution can be produced in high-quality using flash crystallizers. This is significant because the PTA crystals' size and form can have an impact on the characteristics of the polyester resin that is made from them. Second, flash crystallizers have great throughput capabilities. Given that PTA manufacture is a high volume process, this is significant. Thirdly, flash crystallizers use a fair amount of energy. This is significant since the process of producing PTA consumes a lot of energy.

Five crystallizers are used in the procedure to encourage the crystallization of PTA from the reaction mixture. In order to establish ideal circumstances for PTA crystal formation, these crystallizers use cooling techniques such flash evaporation. The temperature dropped as a result of the flash evaporations, which involved lowering the pressure in the crystallizers. The production of PTA crystals was aided by the drop in temperature while impurities were left behind. The residence duration, temperature, and flash evaporation procedures were all optimized in the design of the crystallizers for quick crystal formation and separation.

3.3.6 Centrifuge

A disk centrifuge is a type of centrifuge that separates solids from liquids using a revolving disk. The creation of PTA from CTA can be accomplished using the disk centrifuge, which is a flexible and effective piece of machinery.

Disk centrifuges are used to separate the raw PTA crystals from the mother liquor during the manufacturing of PTA from CTA. To create high-purity PTA, the raw PTA crystals are then cleaned and dried.

The disk centrifuge comprises of a revolving disk that has been punctured with numerous holes. A bowl that holds the separated solids surrounds the disk. Centrifugal force drives the liquid through the pores in the disk. The liquid is released from the centrifuge while the solids are collected in a dish.

A dependable and effective piece of machinery with numerous applications is the disk centrifuge. Because it can effectively separate the raw PTA crystals from the mother liquor, the disk centrifuge is especially well-suited for producing PTA from CTA.

3.3.7 Dryer

An industrial dryer called a rotating steam tube drier uses steam to evaporate moisture from a solid substance. A flexible and effective piece of machinery, the rotary steam tube dryer can be utilized for a variety of tasks, including the creation of PTA from CTA.

The raw PTA crystals are dried in rotary steam tube dryers during the process of producing PTA from CTA. Using a disk centrifuge, the mother liquor is first removed from the crude PTA crystals. The rotary steam tube drier is then fed with the raw PTA crystals.

A spinning drum that is heated by steam is the main component of the rotary steam tube dryer. The interior of the drum is covered in unprocessed PTA crystals. The steam warms the unprocessed PTA crystals while the drum turns. A vacuum device is then used to evaporate and remove the moisture from the raw PTA crystals in the drum.

A dependable and effective piece of machinery with numerous applications is the rotary steam tube dryer. The rotary steam tube dryer's great effectiveness at drying the raw PTA crystals makes it especially well-suited for the production of PTA from CTA.

3.4 Catalyst

Catalysts are essential for improving the selectivity and conversion efficiency of the conversion processes in the synthesis of purified terephthalic acid (PTA) from crude terephthalic acid (CTA). Palladium-coated carbon is one of the catalysts that is frequently employed in the process. In many chemical processes, including the oxidation of aromatic compounds, palladium catalysts have demonstrated exceptional performance.

Palladium coated carbon was selected as a catalyst in the packed bed reactor (PBR) because of its distinct qualities. High catalytic activity, stability, and selectivity are characteristics of palladium. To provide a broad surface area and increase the exposure of active areas, the metal is supported on carbon. Palladium on the carbon surface accelerates the desired conversion processes by facilitating the adsorption of reactant molecules.

The CTA to PTA conversion process benefits greatly from the palladium-coated carbon catalyst. First of all, it offers excellent conversion efficiency, enabling a full conversion of CTA into PTA. The catalyst guarantees that impurities are eliminated and that only pure PTA crystals are produced. It also has good selectivity, allowing for the required reactions while limiting unfavorable side effects. Higher product yields and better product quality results from this.

Palladium-coated carbon catalysts are also renowned for their durability and resistance to deactivation. By ensuring consistent performance during protracted periods of operation, this lowers the requirement for frequent catalyst replacement and raises the process' overall effectiveness. The catalyst is ideal for the particular conditions in the PTA manufacturing since it has a high tolerance to process factors like temperature and pressure.

Numerous studies and pieces of research support the choice of the palladium coated carbon catalyst for the packed bed reactor (PBR). For instance, a study by Zhang et al. (2018) showed the value of palladium catalysts in aromatic chemical hydro purification processes.

CHAPTER 4

MATERIAL AND ENERGY BALANCE

4.1 Material Balance:

The material balance involves tracking the quantities of CTA, water, and other raw materials entering the system and comparing them with the quantities of PTA crystals and byproducts produced. The material balance equations are typically based on the principle of conservation of mass and can be expressed as follows:

Basis: 1-hour steady state operation on an open system

General Material Balance Equation:

Units are (kg/hr)

$$Mass\ In - Mass\ Out + Generation - Consumption = Accumulation$$

$$Incoming\ Mass = Outgoing\ Mass$$

4.2 Energy Balance:

Quantifying the energy inputs, such as heat and steam, and the energy outputs, such as waste heat, constitutes the energy balance. Based on the idea of energy conservation, the energy balance equations have the following form:

$$Energy\ In = Energy\ Out$$

The heat transfer within different unit operations, such as heat exchangers and steam generation, is considered by the energy balance equations. The energy balance equations also consider the energy content of the feed and products as well as the energy needed for chemical processes.

It is feasible to evaluate the general process efficiency, identify potential for improvement, and maximize resource use in the PTA production process by carrying out a thorough material and energy balancing.

4.2.1 Feed Tank

Material Balance:

- 4-CBA – 2500ppm
- Water – 30% Slurry
- Mass In = Mass Out

Table 1: Feed Tank Material Balance

Components	In	Out
TA (kg/hr)	62,586	595.7
Water (kg/hr)	152,982	152,982
4-CBA (kg/hr)	167.9	0.4
P-Toluic Acid (kg/hr)	53.0	205.8
Hydrogen (kg/hr)	13.3	8.9
Total (kg/hr)	215,806.1	215,806.1

Energy Balance:

- $\Delta H = 0$
- Enthalpy In = Enthalpy Out

This equation represents the calculation of the final temperature (T_f). The equation considers the mass flow rates and specific heat capacities of the fluids to determine the final temperature.

$T_f = (m_1c_{p1}t_1 + m_2c_{p2}t_2) / (m_1c_{p1} + m_2c_{p2})$ (Smith, Van Ness, & Abbott, 2005)

T_f: Final temperature of the system

m_1, m_2: Mass flow rates of the fluids

c_{p1}, c_{p2}: Specific heat capacities of the fluids

t_1, t_2: Initial temperatures of the fluids (Smith, Van Ness, & Abbott, 2005)

Table 2: Feed Tank Energy Balance

Feed Tank	**CTA**	**Water**	**Feed Tank Outlet**
Flowrate (kg/hr)	62,586	152,982	215568
Cp (kg)	1.34	4.18	-
Temperature (°C)	80	110	106.86
Pressure (bar)	1.5	1.5	1.5

4.2.2 Pumps

Material Balance:

- Mass In = Mass Out

Energy Balance:

This equation represents the calculation of the work or power output.

$$W = (mV(P2 - P1))/\eta;\ \eta = 80\%$$

W: Work or power output

m: Mass flow rate of the fluid

V: Volume of the fluid

P2, P1: Pressure at the outlet and inlet, respectively

η: Efficiency of the system (given as 80% in the example)

Table 3: Pump 1 Parameters

Pump 1	
Flowrate (kg/hr)	215568
Pressure inlet (bar)	1.5
Pressure outlet (bar)	10.5
Specific volume (m^3/kg)	0.000899
Work in (kJ)	1543.24

Table 4: Pump 2 Parameters

Pump 2	
Flowrate (kg/hr)	215568
Pressure inlet (bar)	10.5
Pressure outlet (bar)	80
Specific volume (m^3/kg)	0.000899
Work in (kJ)	11917.3

4.2.3 Pre-Heater

Material Balance:

- Mass In = Mass Out

Energy Balance:

$$Q = mC\ (\mathrm{Tf} - \mathrm{Ti})$$

$$Steam\ Required = Q/\boldsymbol{\lambda}$$

Q: Heat transfer or energy transferred to or from the system

m: Mass flow rate of the fluid

Cp: Specific heat capacity of the fluid

Tf: Final temperature of the fluid or system

Ti: Initial temperature of the fluid or system

λ: latent heat of vaporization

Table 5: Heat Exchanger 1

PRE-HEATER 1		
Components	In	Out
T (°C)	106.7	126.2
Cp (Avg)	3.35	-
m (kg)	215568	-
ΔT (°C)	19.5	-
Q (kJ)	9,887,526.2	-
λ (from C3) (kJ/kg)	1971.6	-
Steam Required (kg)	5036.9	-

Table 6: Heat Exchanger 2

PRE-HEATER 2		
Components	In	Out
T (°C)	126.2	144.9
Cp (Avg)	3.507	-
m (kg)	215568	-
ΔT (°C)	18.6	-
Q (kJ)	10,025,615.2	-
λ (from C2) (kJ/kg)	1869.1	-
Steam Required (kg)	5358.4	-

Table 7: Heat Exchanger 3

PRE-HEATER 3		
Components	In	Out
T (°C)	144.9	200.5

Cp (Avg)	3.64	-
m (kg)	215568	-
ΔT (°C)	55.5	-
Q (kJ)	30850906.6	-
λ (from C1) (kJ/kg)	1761.0	-
Steam Required (kg)	17519.4	-

Table 8: Heat Exchanger 4

PRE-HEATER 4		
Components	In	Out
T (°C)	200.5	235
Cp (Avg)	3.7	-
m (kg)	215568	-
ΔT (°C)	34.5	-
Q (kJ)	2822885.6	-
Steam Required (kg)	20406.6	-

Table 9: Heat Exchanger 5

PRE-HEATER 5		
Components	In	Out

T (°C)	235	283
Cp (Avg)	3.92	-
m (kg)	215568	-
ΔT (°C)	48	-
Q (kJ)	26930328.3	-
Steam Required (kg)	20406.6	-

4.2.4 Reactor

Material Balance:

- Steady state operation
- Mass Out = Mass in + Generation – Consumption

Reaction:

4-CBA + $2H_2$ → P-Toluic Acid + H_2O

4-CBA conc. in feed: 2500ppm & 4-CBA conc. required at outlet: 25ppm

HP steam is used to heat H_2 gas.

Energy Balance:

Hout = Hin + m4−cba. Hrxn

Since m4−cba is in such a tiny amount;

Hin ≈ Hout & Tin ≈ Tout ≈ 283°C

Table 10: Reactor Material Balance

Components	Feed (kg/hr)	Mass Consumed (kg/hr)	Mass Generated (kg/hr)	Reactor Outlet (kg/hr)
TA	62,586	-	-	62,586
P-Toluic Acid	53.9	-	151.9	205.8

4-CBA	167.9	167.5	-	0.4
H_2O	152,982	-	-	152,982
Hydrogen	13.3	8.9	4.3	-
Total	215,803.1	176.4	156.2	215,803.1
Temperature (°C)	283	-	-	283
Pressure (bar)	82	-	-	82

4.2.5 Crystallizer

Material Balance:

- Mass In = Mass of water ejected as vapor + Mass of liquid at outlet
- T = Tsat at the pressure of crystallizer

Simultaneous Material & Energy Balance:

Mass of Vapor Vented through: Flashing at saturation conditions

- Mass of water * Quality
- Quality = (H inlet – H at sat conditions)/Latent Heat

Heat evolved from Crystallization:

- Mass of crystals formed * Heat of crystallization

Table 11: Crystallizers Material Balance

Components	To C1	C1-V	C1-L	C2-V	C2-L	C3-V	C3-L	C4-V	C4-L	C5-V	C5-L
TA (kg/hr)	45,662	-	8219.2	-	2,926.03	-	1,302.1	-	533.86	-	170.8
Water (kg/hr)	106,825	17,519.4	89,306.1	5,358.4	83,947.7	5,036.9	78,910.8	3,156.4	75,754.37	3,406.9	72,345.4
4-CBA (kg/hr)	1.098	-	1.098	-	1.098	-	1.098	-	1.098	-	1.098
P-TA (kg/hr)	107.3	-	107.25	-	107.25	-	107.25	-	107.25	-	107.25
TA solid (kg/hr)	-	-	37,442.9	-	5293.2	-	1623.9	-	768.24	-	363.02
H2 (kg/hr)	-	-	-	-	-	-	-	-	-	-	-

Total (kg/hr)	152596	17,519.4	97,633.6	5,358.4	86,982.1	5,036.9	80,321.3	3,156.4	76,396.6	3,406.9	72,624.6
Heat Evolved (kJ)	-	4,596,494.1		649,787.1		199,356.1		94,309.1		44,564.3	
Crystallizer Efficiency %	-	82		64.47		55.51		59		68	
λ (kJ/kg)	-	1761.03		1869.1		1971.6		-		-	
Temp (°C)	283	244		218		185		170		152	
Pressure (bar)	82	33		21		12		7.7		4	

Table 12: Efficiency of Crystallizer 1: 82% (Data from Lotte Chemicals)

Data	Feed	Outlet
Mass Crystallized (kg)	-	37,442.9
Heat of Crystallization (kJ/kg)	122.8	-
Heat Evolved (kJ)	-	4,596,494.1
Total Vapor Formed (kg)	-	17,519.4
Latent Heat of Steam (kJ/kg)	-	1,767.03
Enthalpy Upstream of Steam (At Pressure) (kJ/kg)	1,331.4	-
Enthalpy Downstream of Steam (At Pressure) (kJ/kg)	-	1,041.9
Temperature (°C)	283	244
Pressure (bar)	82	33

4.2.6 Centrifuge

Material Balance:

- Mass In = Mass Out
- **90%** separation of water from feed occurs
- The separated liquid is sent to the oxidation plant as recycle.

Energy Consumption = 716.2 kWh

Table 13: Centrifuge Material Balance

Components	To Centrifuge	Recycle	Dryer
TA (kg/hr)	572.7	572.7	-
Water (kg/hr)	92,546.9	83,292.21	9,254.69
4-CBA (kg/hr)	0.4	-	0.4
P-TA (kg/hr)	179.7	161.73	17.97
TA solid (kg/hr)	62,013.3	-	62,013.3
Total (kg/hr)	155,313.4	84,026.64	71,286.36
Temperature (°C)	152	99.6	

4.2.7 Dryer

Material Balance:

- Inlet + production = Outlet + Accumulation
- Dryer Efficiency = 99.90%

Table 14: Dryer Material Balance

Components	In Dryer	Moisture removed	Product
TA liquid (kg/hr)	-	-	-
Toluic Acid (kg/hr)	17.97	-	17.97
4-CBA (kg/hr)	0.4	-	0.4
Water (kg/hr)	9,254.69	9162.14	92.54
TA crystals (kg/hr)	62,013.3	-	62,013.3
Total Amount (kg/hr)	71,286.36	9162.14	62.122.22
Temp (°C)	99.6	105	105

Energy Balance:

- Q = Sensible + Latent heat
- Steam Required = Q/λ

- λ = Latent heat of steam used for heating
-

Table 15: Dryer Energy Balance

Components	Feed	Moisture Removed	Out
Temperature (°C)	99.6	105	105
Water (kg/hr)	7169.4	-	7.2
Vapor (kg/hr)	-	7162.3	-
Q sensible (kJ)	11975.3		
Q latent (kJ)	16186719.8		
Q total (kJ)	16198695.1		
Steam required (kg)	7767.6		

CHAPTER 5

EQUIPMENT DESIGN

5.1 Composition List

5.1.1 Shell and Tube geometrical design Considerations

1. Tube Layout and Size: The tube layout and size must be meticulously chosen to provide sufficient heat transfer area and to accommodate the desired fluid flow rates. Tube diameter, length, and pitch have an effect on heat transfer performance and pressure decrease.
2. Baffles and passes: Baffles are used to improve heat transfer by directing fluid flow and generating turbulence. Overall heat transfer coefficient and pressure drop are affected by the number and design of baffles, as well as the configuration of multiple tube passes.
3. Shell side: The design should take into account the fluid properties, flow rates, and pressure decrease on the shell side. Heat transfer efficacy is affected by the selection of shell-side baffles, inlet and outlet configurations, and flow arrangements (such as parallel or counter-flow).
4. Material Selection: Appropriate material selection is necessary to assure compatibility with the process fluids, temperature, and pressure conditions, and to prevent corrosion, erosion, and fouling.

5.1.2 Kern’s Method

Shell and tube heat exchanger design using Kern's method follows a systematic approach to determine the required heat transfer area and size of the heat exchanger appropriately. The method involves several steps:

1) Determine the Overall Heat Transfer Coefficient (U):

- Calculate the individual heat transfer coefficients for the hot and cold fluids inside the shell and tubes based on their properties, flow conditions, and heat transfer mechanisms (convection, conduction).
- Consider fouling factors to account for any surface fouling that may reduce the heat transfer coefficients.
- Calculate the overall heat transfer coefficient (U) using the appropriate equation, such as the Kern method equation for shell and tube heat exchangers.

2) Determine the Logarithmic Mean Temperature Difference (LMTD):
   - Identify the temperature profiles of the hot and cold fluids at the inlet and outlet of the heat exchanger.
   - Calculate the temperature differences between the fluids at each end and determine the logarithmic mean temperature difference (LMTD) using the appropriate equation based on the flow arrangement (parallel, counter-flow, or crossflow) and the number of shell and tube passes.

3) Determine the Required Heat Transfer Area:
   - Calculate the required heat transfer area (A) using the equation:
     $Q = U \times A \times LMTD$
     where Q is the heat duty or the desired heat transfer rate.
   - Rearrange the equation to solve for the required heat transfer area (A):
     $A = Q \div (U \times LMTD)$

4) Perform Iterative Sizing Calculations:
   - Estimate the initial heat exchanger dimensions and configuration based on the required heat transfer area.
   - Calculate dimensions, considering tube diameter, tube length, number of tubes, and overall dimensions.

- Identifying and calculating the baffle type and spacing.
- Calculate and verify that the pressure decrease across the heat exchanger meets the design specifications.
- If necessary, iterate the sizing calculations to obtain an optimal design.
- The tube side fluid is the CTA mixed to be heated.
- The shell side fluid is the saturated steam from the second crystallizer C-103.

Stream Properties:

- E-101

Table 16: Stream Properties in E-101

Cold Fluid - Tube Side		Hot Fluid - Shell Side	
Parameters	**Value**	**Parameters**	**Value**
Inlet Temperature (°C)	110	Inlet T (°C)	184.21
Outlet T (°C)	170	Outlet T (°C)	184.21
Mass flowrate (kg/hr)	209966	Mass Flowrate (kg/hr)	24000
Avg. Cp (kJ/kg.K)	1.2093	Cp (kJ/kg.K) vapor	1998.55
Avg. density (kg/m^3)	907.62	Density (kg/m^3) vapor	5.22
Avg. viscosity (Cp)	0.251	Viscosity (Cp) vapor	0.0158

Thermal conductivity (W/mK)	0.6804	Thermal Conductivity (W/mK)	0.0323

Calculated Parameters:

- E-101

Table 17: E-101 Design Parameters

Parameters	Tube Side	Shell Side
Duty (MW)	13.425	
LMTD (°C)	35.84	
Reynold number	166205.8	142024.4
Prandtl number	1.7	0.94
h (film coefficient)	17061.2	15747.2
Uc (W/m^2K)	3014.3	
Ud (W/m^2K)	2318.5	
Rd (m^2K/W)	0.0001	
Area (m^2)	161.4	
Pressure Drop (kPa)	165.105	40.447

- The exchanger geometry was chosen based on Aspen Exchanger Design and Rating (EDR) recommendation.
- The design was modified considering operation warnings provided by EDR.

Tube and Shell Side Geometries

Table 18: E-101 Tube-Side Geometry

Tube Side	
Number	270
Length (m)	10.2
OD (m)	0.019
ID (m)	0.0132
Pitch	Triangular
Passes	2
Material	Stainless Steel

Table 19: E-101 Shell-Side Geometry

Shell Side	
OD (m)	0.5895
ID (m)	0.58
Baffle spacing (m)	0.3
Passes	1
Material	Stainless Steel

The heat exchanger layout as generated EDR is given below based on the above design.

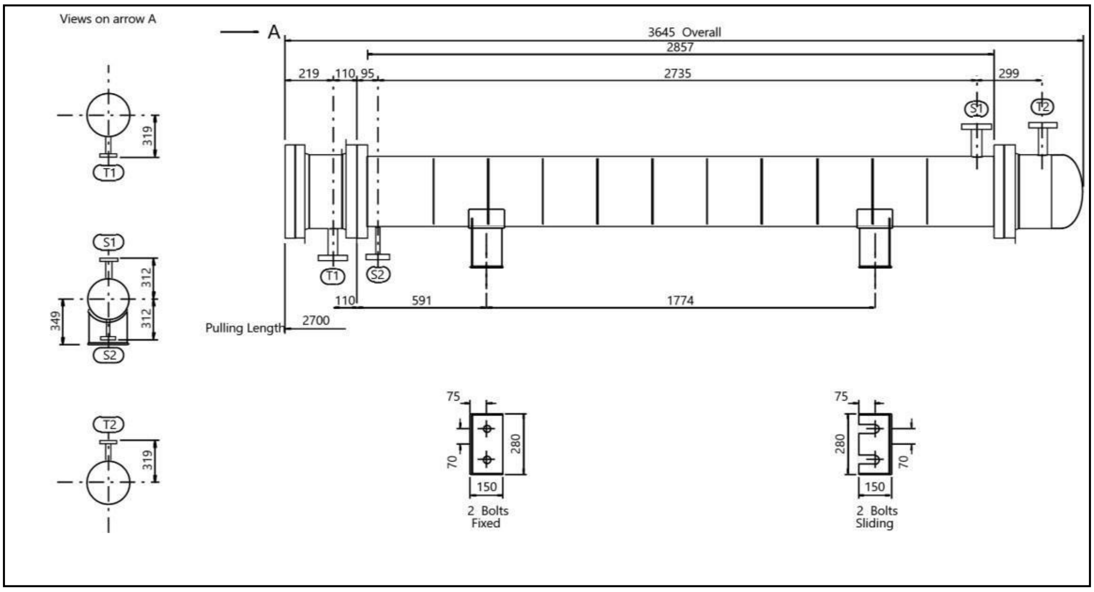


Figure 4: EDR Generated E-101 Layout

5.2 Packed-Bed Reactor Design

A typical Packed Bed Reactor is shown and the some of the design considerations are described:

1. Catalyst Bed Design: The design should take into account the selection of an appropriate catalyst and its injection density within the reactor. The height, diameter, and void fraction of the bed influence the reaction kinetics, pressure decrease, and heat transfer efficiency.
2. Configuration of the Reactor: The configuration of the reactor, such as fixed-bed, fluidized-bed, or trickle-bed, is determined by the specific reaction requirements. Limitations on catalyst retention, heat transmission, and mass transfer are specific to each configuration.
3. Flow Distribution: Appropriate distribution of reactants and uniform flow across the catalyst bed are essential for efficient reaction and prevention of hot areas. The design must integrate appropriate distributor plates or devices to guarantee uniform flow distribution.

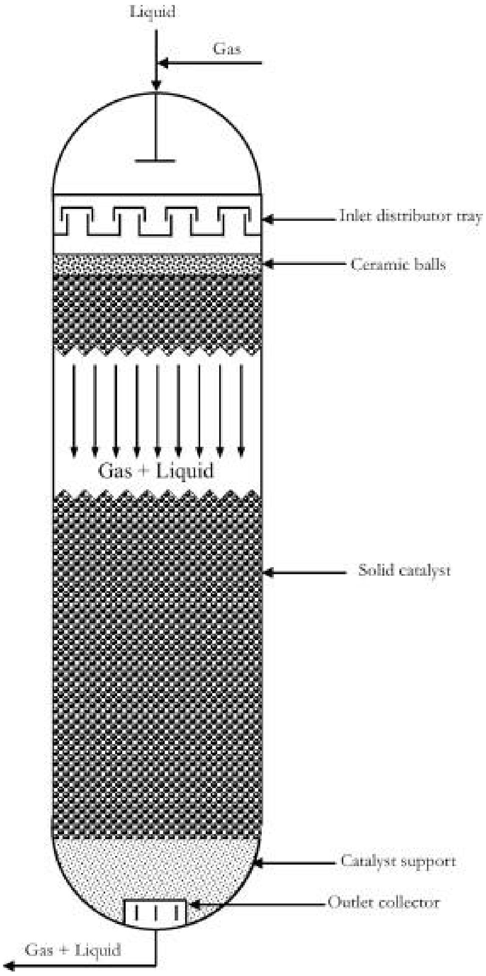


Figure 5: PBR Reactor R-101

4. Temperature and Pressure Control: The design of the reactor should accommodate for the use of heat transfer fluids, cooling jackets, or external heating systems for temperature control. Also, to be considered are pressure control measures, such as safety valves and pressure relief systems.

5.2.1 Procedure for Packed-bed Reactor Design Calculations:

Following are the PBR calculation steps:

Reaction Kinetics and Rate Equation:

- Identify the desired reaction and derive the rate equation representing the relationship between reactant concentrations, catalyst concentrations, and reaction rate.
- If necessary, conduct experimental studies or consult scientific literature to determine kinetic parameters such as reaction rate constants and reaction orders.

Mass balance:

- Develop the overall mass balance equation for the PBR, taking into account the reaction stoichiometry, input flow rates, and reactant conversions.
- Take into account any possible adverse or competing reactions.
- Calculation of Residence Time:
- Determine the weight of catalyst necessary in the PBR to accomplish the desired level of conversion.
- Determine the residence time when employing a PBR model based on the reaction kinetics and desired conversion.

Pressure drop calculation:

- Estimate the pressure drop across the PBR by considering the flow rates, bed height, particle size distribution, and bed void fraction.
- Utilize the Ergun Equation to calculate the pressure drop.
- Considerations for Heat Transfer:
- Evaluate the heat transfer requirements, particularly in exothermic reactions, to prevent temperature rise and preserve desired reaction conditions.
- Determine whether additional heat transfer surfaces, such as cooling coats or internal coils, are required to regulate the temperature of the reactor.

Reactor Sizing:

- Determine the bed height and diameter of the PBR based on the desired conversion, reaction kinetics, pressure drop limitations, and heat transfer considerations.
- Include in the sizing calculations variables such as catalyst loading, particle size, and bed vacancy fraction.
- As more impure TA is refined, the effectiveness of the catalyst decreases. The end of the catalyst's useful life is determined by the quality of the Pure TA product and the required reactor pressure.
- Utilize Aspen to obtain concentration profiles.

Safety Precautions:

- Conduct hazard and risk assessments to evaluate safety aspects, including potential temperature and pressure excursions.
- Implement safety measures to ensure secure operation, such as relief systems or interlocks.

5.2.2 Reactions:

The following reactions occur in series to convert 4-CBA to p-toluic acid by reacting with hydrogen gas.

$$C_8H_6O_3 + H_2 \longrightarrow C_8H_8O_3$$

$$C_8H_8O_3 + H_2 \longrightarrow C_8H_8O_2 + H_2O$$

Reaction kinetics:

$$; r_1 = 0.047 \exp\left(-\frac{16976.4}{RT}\right) C_{4-CBA}^{0.96} C_{H_2}^{0.24}$$

$$; r_2 = 0.153 \exp\left(-\frac{23438.6}{RT}\right) C_{4-HMBA}^{0.61} C_{H_2}^{0.75}$$

- Based on the reaction kinetics and operating conditions, weight of catalyst is calculated.

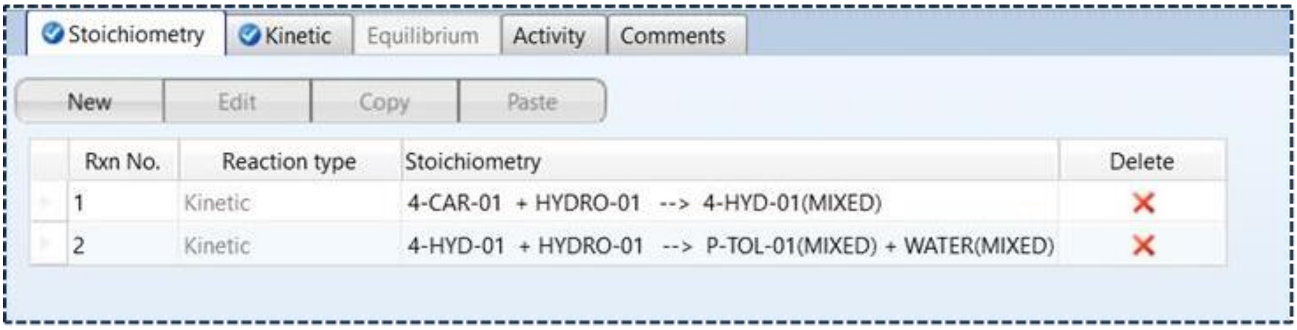
- Aspen Plus was used to find the amount of catalyst mass required for the desired conversion.

Operating Conditions:

Table 20: Operating Conditions R-101

Parameter	Value
Temperature (°C)	283
Pressure (bar)	82
Feed Flowrate (kg/hr)	215,749
H2 Flowrate (kg/hr)	13.3
4-CBA feed concentration (ppm)	2500
Catalyst	0.5% (Pd/C)
Bulk density (kg/m3)	475

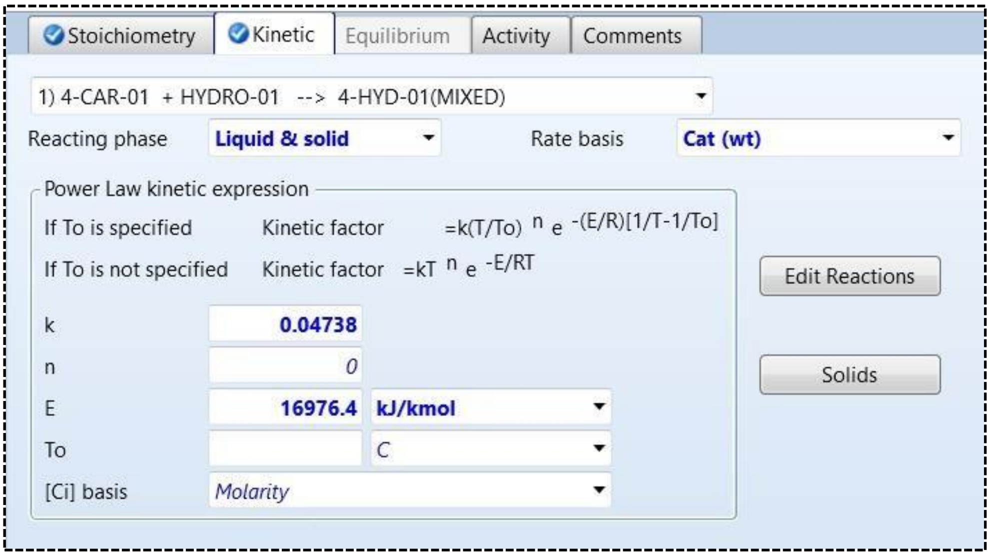
Reaction sets were defined in Aspen Plus based on reaction kinetics data.



Rxn No.	Reaction type	Stoichiometry	Delete
1	Kinetic	4-CAR-01 + HYDRO-01 --> 4-HYD-01(MIXED)	✗
2	Kinetic	4-HYD-01 + HYDRO-01 --> P-TOL-01(MIXED) + WATER(MIXED)	✗

Figure 6: Reaction Sets In Aspen Plus

Reaction 1:



1) 4-CAR-01 + HYDRO-01 --> 4-HYD-01(MIXED)

Reacting phase: **Liquid & solid**

Rate basis: **Cat (wt)**

Power Law kinetic expression

If To is specified Kinetic factor $=k(T/To)^{n} e^{-(E/R)[1/T-1/To]}$

If To is not specified Kinetic factor $=kT^{n} e^{-E/RT}$

k: **0.04738**

n: *0*

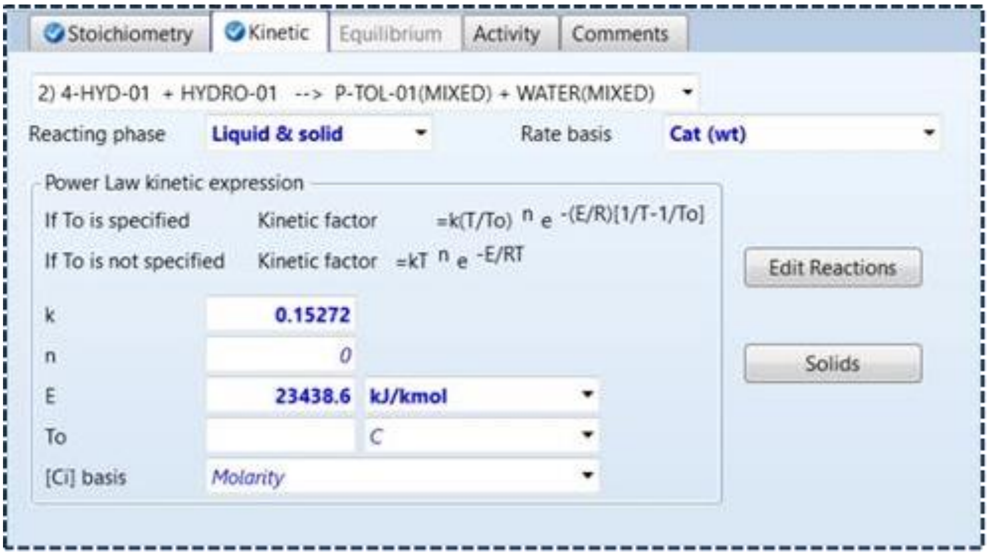
E: **16976.4** **kJ/kmol**

To: C

[Ci] basis: *Molarity*

Figure 7: Rxn-1

Reaction 2:



2) 4-HYD-01 + HYDRO-01 --> P-TOL-01(MIXED) + WATER(MIXED)

Reacting phase: **Liquid & solid**

Rate basis: **Cat (wt)**

Power Law kinetic expression

If To is specified Kinetic factor $=k(T/To)^{n} e^{-(E/R)[1/T-1/To]}$

If To is not specified Kinetic factor $=kT^{n} e^{-E/RT}$

k: **0.15272**

n: *0*

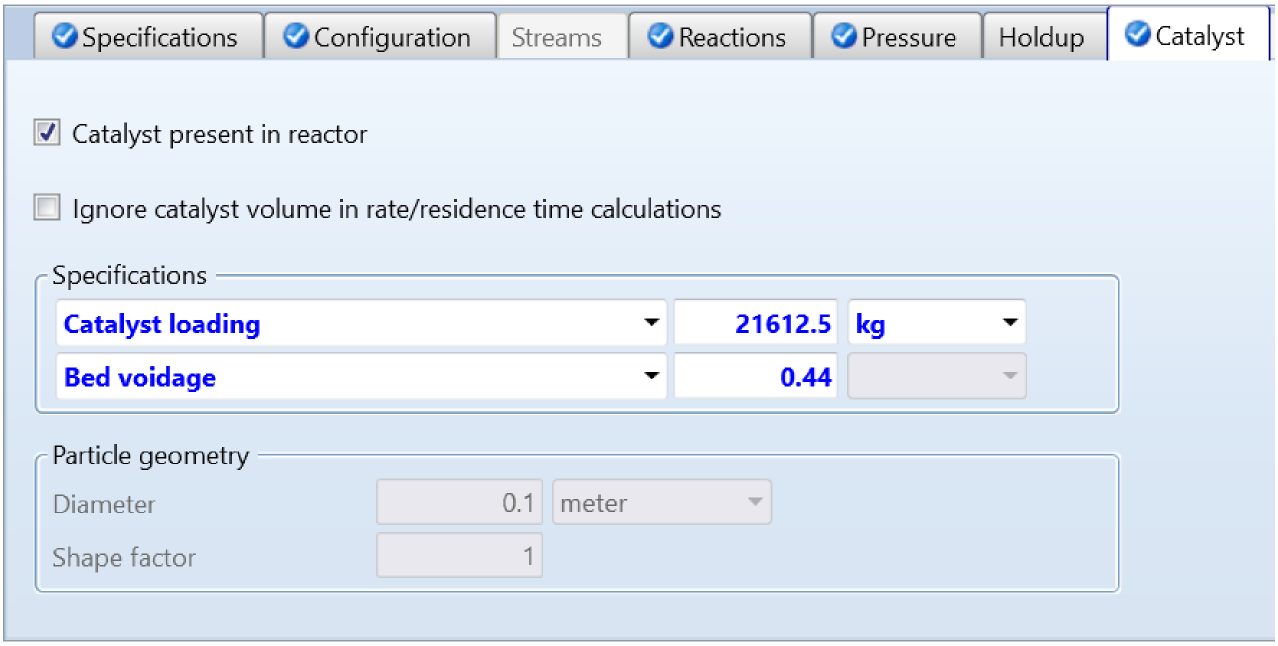
E: **23438.6** **kJ/kmol**

To: C

[Ci] basis: *Molarity*

Figure 8: Rxn-2

- Catalyst weight (W) was then determined based on conversion desired.



☑ Catalyst present in reactor

☐ Ignore catalyst volume in rate/residence time calculations

Specifications

Catalyst loading	**21612.5**	**kg**
Bed voidage	**0.44**	

Particle geometry

Diameter	0.1	meter
Shape factor	1	

Figure 9: Catalyst Input in Reactor

Calculations

Equations used:

- $Vb = \frac{W}{\rho_b}$
- $Vr = 1.2\,Vb$
- $Vv = Vd + Vr$
- $\frac{L}{D} = 2.6$
- $D = \sqrt[3]{\frac{2Vr}{\pi}}$

Where

Vr: volume of bed

Vr: volume of reactor

Vd: volume of dissolver

Vv: volume of vessel

Table 21: R-101 Specification

Parameter	Value
Weight of Catalyst (kg)	21,613
Volume of Catalyst Bed (m^3)	45.5
Volume of reactor (m^3)	54.6
Volume of Dissolver (m^3)	17.3
Volume of Vessel (m^3)	71.9
Length (m)	7.4
Diameter (m)	2.8

5.3 Crystallizer

5.3.1 Crystallizer design Considerations

A typical crystallizer is shown with some design considerations given below:

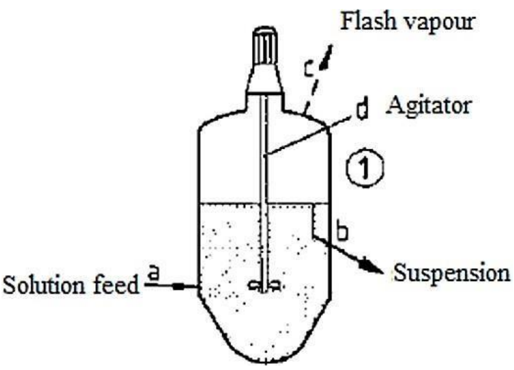


Figure 10: General Crystallizer Schematic

1. Crystallization Method: The selection of an appropriate crystallization method, such as cooling crystallization, evaporation crystallization, or anti-solvent crystallization, is contingent on the process requirements and desired crystal properties.
2. Mixing and agitation: Effective mingling and agitation ensure uniform solute distribution, regulate supersaturation, and promote crystal growth. The design should include suitable mixing mechanisms, such as impellers, to accomplish the desired levels of agitation.
3. Cooling or heating system: The design should take into account the refrigeration or heating system required to control the crystallization temperature. This may involve the use of heating coils, chilling water, or refrigerants.
4. Crystallizer configuration: various crystallizer configurations, such as draft tube, stirred tank, and crystallizer with internals, offer various advantages based on the desired crystal characteristics and process requirements.

5.3.2 Procedure for Crystallizer Design Calculations:

1. **Solubility Data:**
    - Gather solubility data for the solute in the solvent at different temperatures and concentrations.
    - The table used for solubility data is shown below.

Table 21: Solubility Data od Crystallizer C-101

Temperature (^{0}C)	Solids Strength (%)
200	1.77
220	3.85
240	8.25
250	11.75
260	16.67
261	17.35
262	17.83
263	18.37
264	19.03
265	19.68
266	20.32
267	20.95
268	21.57
269	22.18
270	23.08
271	23.66
272	24.24
273	25.09
274	25.92
275	26.74
276	27.54

277	28.32
278	29.08
279	30.07
280	30.08
281	31.74
282	32.43
283	33.34
284	34.43
285	35.28
286	36.1
287	37.1
288	38.27
289	39.02
290	40.12

2. Crystal Growth Kinetics:

- Understand the crystal growth kinetics of the solute in the solvent, such as the growth rate and nucleation rate. This information can be obtained from literature or experimental data.
    - $G = k_g e^{-\frac{E_a}{RT}} (C - C_{eq})^g$

3. Residence Time:

- Based on the average crystal growth rate, the residence time is calculated which yields the required volume
    - $\tau = \frac{Lc}{6G}$
    - $V_{req} = Q\tau$
    - $V_{tank} = \frac{Vreq}{0.6}$

- Flash Evaporation is used to crystallize terephthalic acid.
- This leaves the liquid p-toluic acid in the mother liquor.
- The saturated flash steam is used as heating medium for the feed.

Operating Conditions:

Table 22: Operating Conditions of Crystallizer C-101

Parameters	Value
Temperature (°C)	283
Pressure (bar)	82
Feed flowrate (kg/hr)	152,596
Vapor flowrate (kg/hr)	17,519
Liquid flowrate (kg/hr)	97,634
Volumetric liquid flowrate (m^3/hr)	128.5

- The crystallizer residence time is determined by the average crystal growth rate (G) which is given by:

$$G = k_g e^{-\frac{E_a}{RT}} (C - C_{eq})^g$$

- The values for the equation parameters are tabulate.

Crystallization Parameters:

Table 23: Process Crystallization Parameters

Parameters	Value
kg (um/s)	1.7251
Ea/R (K)	1763.7
g (constant)	0.984
Concentration	0.3
Equilibrium conc. (C_{eq})	0.00251
Dominant crystal size (mm)	0.2
Avg. Growth rate (m/s)	7.934E-09

- Based on the average crystal growth rate, the residence time is calculated which yields the required volume.

- $V_{req} = Q\tau$ (V_{req} is the required volume)
- $V_{tan} = \frac{Vreq}{0.6}$ (V_{tank} is the tank volume)
- $\tau = \frac{L_c}{6G}$ (τ is the residence time & L_c crystal size)

Crystallizer Parameters:

Table 24: C-101 Parameters

Parameter	Value
Tank residence time (hr)	0.54
Volume required (m3)	69.4
Volume of vessel (m3)	115.7
Diameter (m)	4

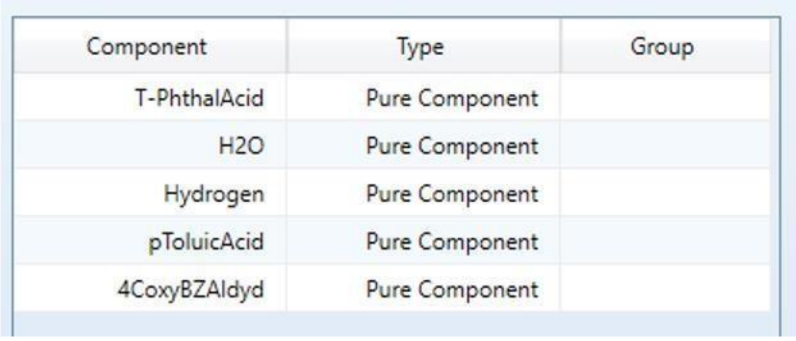
Length (m)	9.2
Level (%)	0.54

CHAPTER 6

PROCESS SIMULATION

6.1 Simulation – HYSYS:

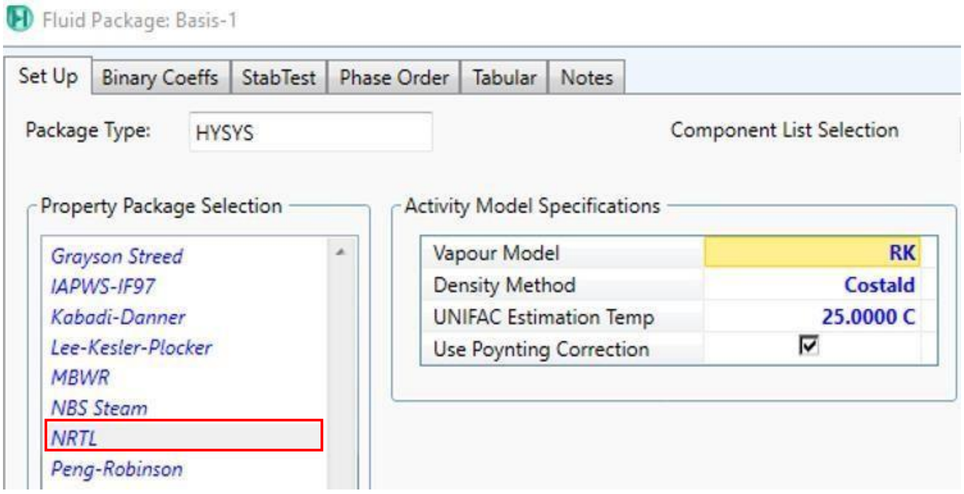
6.1.1 Component List



Component	Type	Group
T-PhthalAcid	Pure Component	
H2O	Pure Component	
Hydrogen	Pure Component	
pToluicAcid	Pure Component	
4CoxyBZAldyd	Pure Component	

Figure 11 Components List in Aspen HYSYS Simulation

6.1.2 Fluid Package

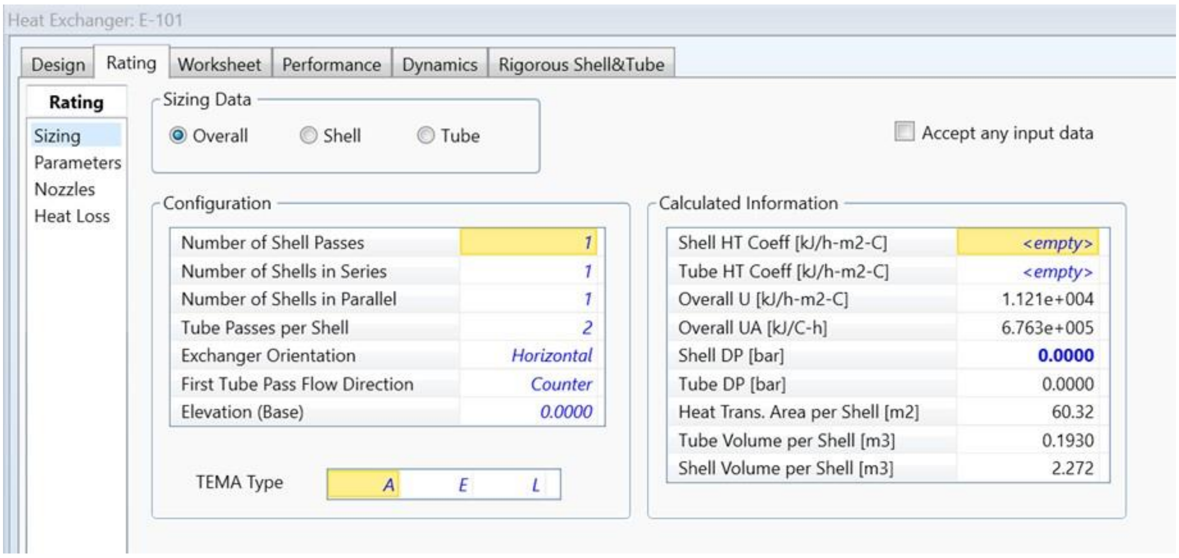


Package Type: HYSYS

Vapour Model	RK
Density Method	Costald
UNIFAC Estimation Temp	25.0000 C
Use Poynting Correction	☑

Figure 12 Fluid Package in Aspen HYSYS Simulation

6.1.3 E-101 Parameters



Sizing Data

● Overall ○ Shell ○ Tube

☐ Accept any input data

Configuration

Number of Shell Passes	1
Number of Shells in Series	1
Number of Shells in Parallel	1
Tube Passes per Shell	2
Exchanger Orientation	Horizontal
First Tube Pass Flow Direction	Counter
Elevation (Base)	0.0000

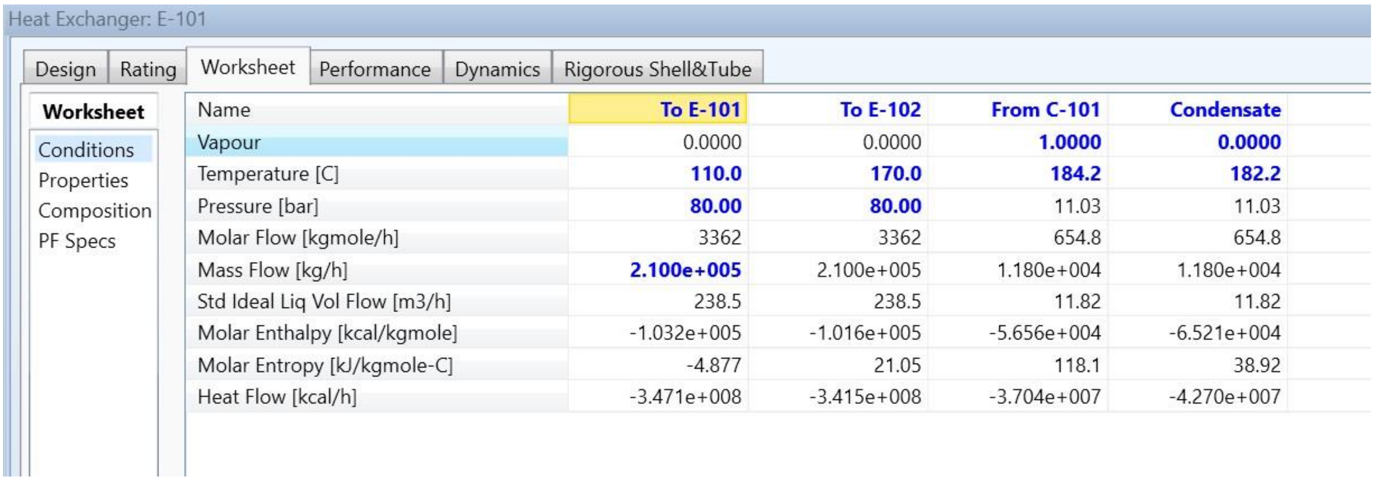
TEMA Type A E L

Calculated Information

Shell HT Coeff [kJ/h-m2-C]	<empty>
Tube HT Coeff [kJ/h-m2-C]	<empty>
Overall U [kJ/h-m2-C]	1.121e+004
Overall UA [kJ/C-h]	6.763e+005
Shell DP [bar]	0.0000
Tube DP [bar]	0.0000
Heat Trans. Area per Shell [m2]	60.32
Tube Volume per Shell [m3]	0.1930
Shell Volume per Shell [m3]	2.272

Figure 13 E-102 Parameters

6.1.4 E-101 Worksheet

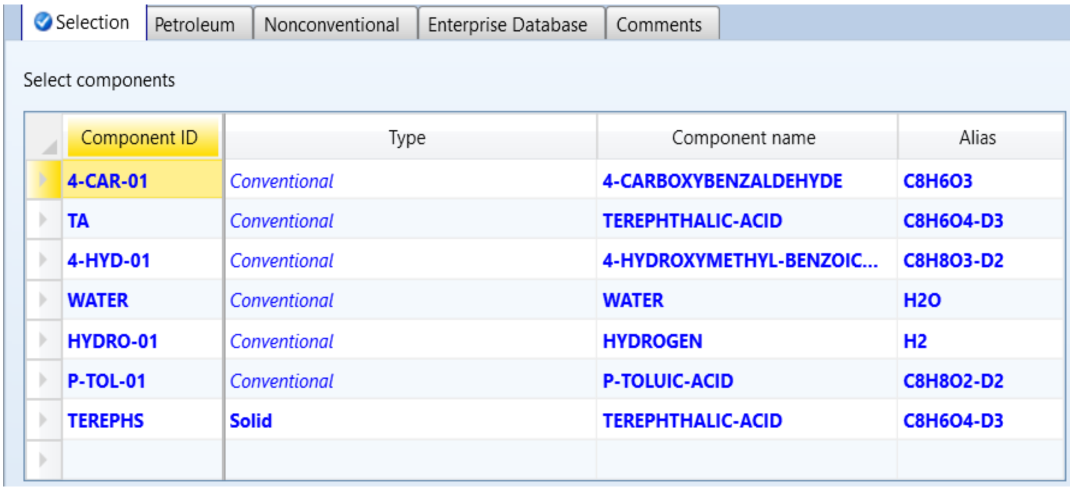


Name	To E-101	To E-102	From C-101	Condensate
Vapour	0.0000	0.0000	1.0000	0.0000
Temperature [C]	110.0	170.0	184.2	182.2
Pressure [bar]	80.00	80.00	11.03	11.03
Molar Flow [kgmole/h]	3362	3362	654.8	654.8
Mass Flow [kg/h]	2.100e+005	2.100e+005	1.180e+004	1.180e+004
Std Ideal Liq Vol Flow [m3/h]	238.5	238.5	11.82	11.82
Molar Enthalpy [kcal/kgmole]	-1.032e+005	-1.016e+005	-5.656e+004	-6.521e+004
Molar Entropy [kJ/kgmole-C]	-4.877	21.05	118.1	38.92
Heat Flow [kcal/h]	-3.471e+008	-3.415e+008	-3.704e+007	-4.270e+007

Figure 14: E-102 Worksheet

6.2 Simulation – Aspen Plus:

6.2.1 Component List

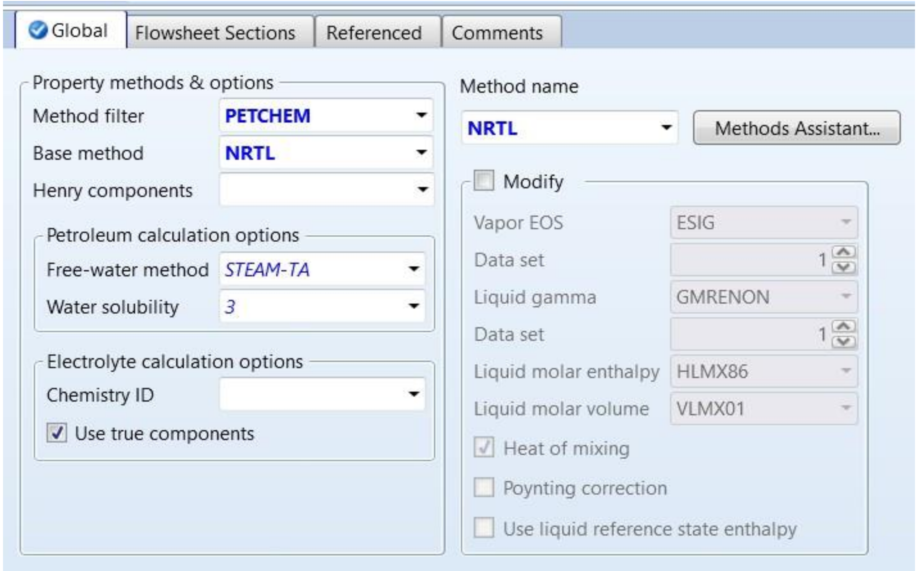


Select components

Component ID	Type	Component name	Alias
4-CAR-01	Conventional	4-CARBOXYBENZALDEHYDE	C8H6O3
TA	Conventional	TEREPHTHALIC-ACID	C8H6O4-D3
4-HYD-01	Conventional	4-HYDROXYMETHYL-BENZOIC...	C8H8O3-D2
WATER	Conventional	WATER	H2O
HYDRO-01	Conventional	HYDROGEN	H2
P-TOL-01	Conventional	P-TOLUIC-ACID	C8H8O2-D2
TEREPHS	Solid	TEREPHTHALIC-ACID	C8H6O4-D3

Figure 15: Components List in Aspen Plus Simulation

6.2.2 Fluid Package



Property methods & options

Method filter: PETCHEM

Base method: NRTL

Henry components:

Petroleum calculation options

Free-water method: *STEAM-TA*

Water solubility: *3*

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Method name: NRTL

☐ Modify

Vapor EOS: ESIG

Data set: 1

Liquid gamma: GMRENON

Data set: 1

Liquid molar enthalpy: HLMX86

Liquid molar volume: VLMX01

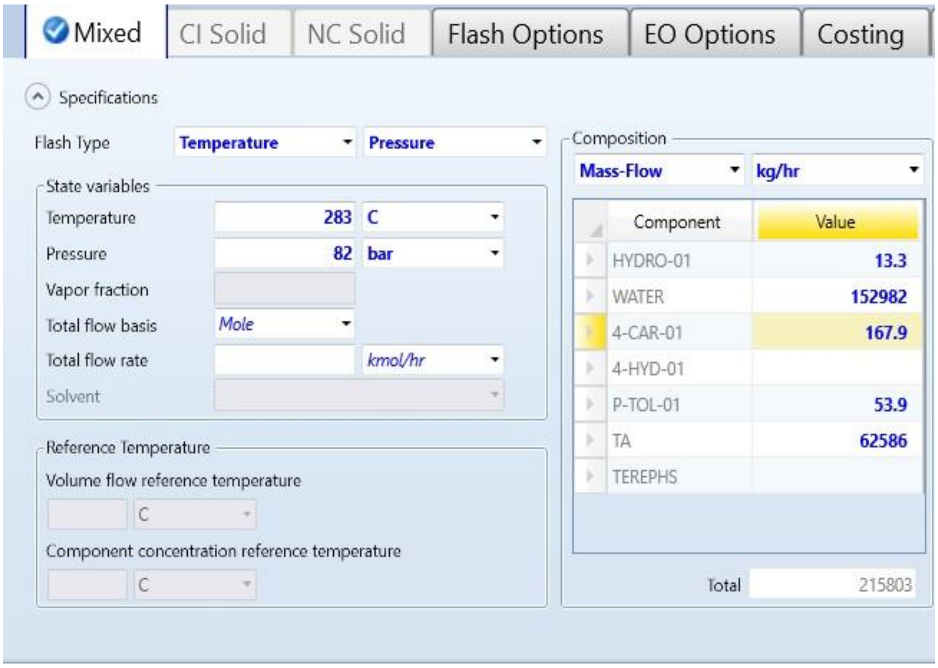
☑ Heat of mixing

☐ Poynting correction

☐ Use liquid reference state enthalpy

Figure 16: Fluid Package in Aspen Plus Simulation

6.2.3 Reactor Inlet Stream



Flash Type: Temperature, Pressure

State variables

Temperature: 283 C

Pressure: 82 bar

Vapor fraction:

Total flow basis: *Mole*

Total flow rate: *kmol/hr*

Solvent:

Reference Temperature

Volume flow reference temperature: C

Component concentration reference temperature: C

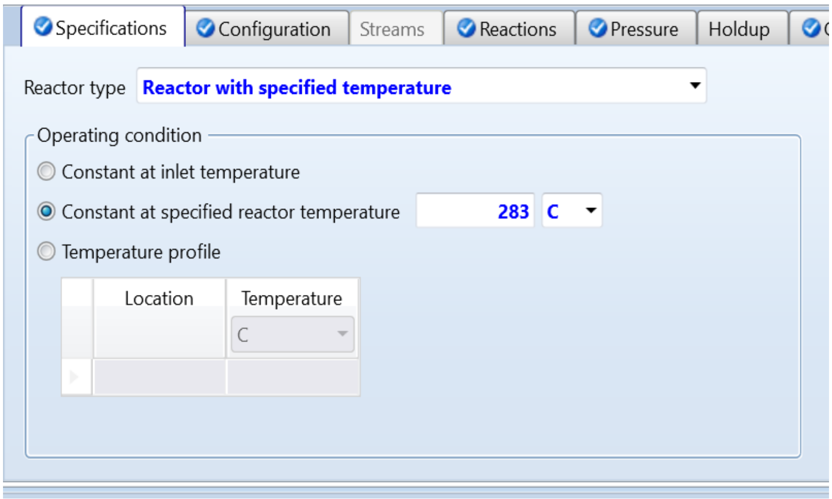
Composition: Mass-Flow, kg/hr

Component	Value
HYDRO-01	13.3
WATER	152982
4-CAR-01	167.9
4-HYD-01	
P-TOL-01	53.9
TA	62586
TEREPHS	

Total: 215803

Figure 17: Reactor Inlet Stream in Aspen Plus Simulation

6.2.4 Reactor Specification



Reactor type: Reactor with specified temperature

Operating condition

○ Constant at inlet temperature

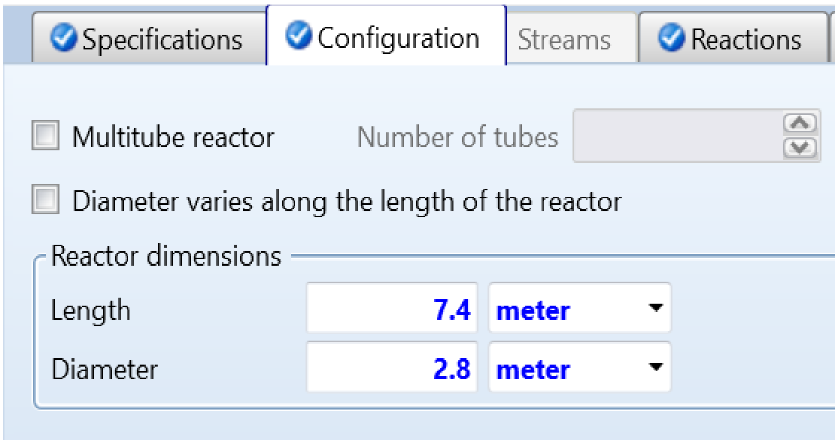
● Constant at specified reactor temperature 283 C

○ Temperature profile

Location	Temperature C

Figure 18: Reactor Specification in Aspen Plus Simulation

6.2.5 Reactor Results



☐ Multitube reactor Number of tubes

☐ Diameter varies along the length of the reactor

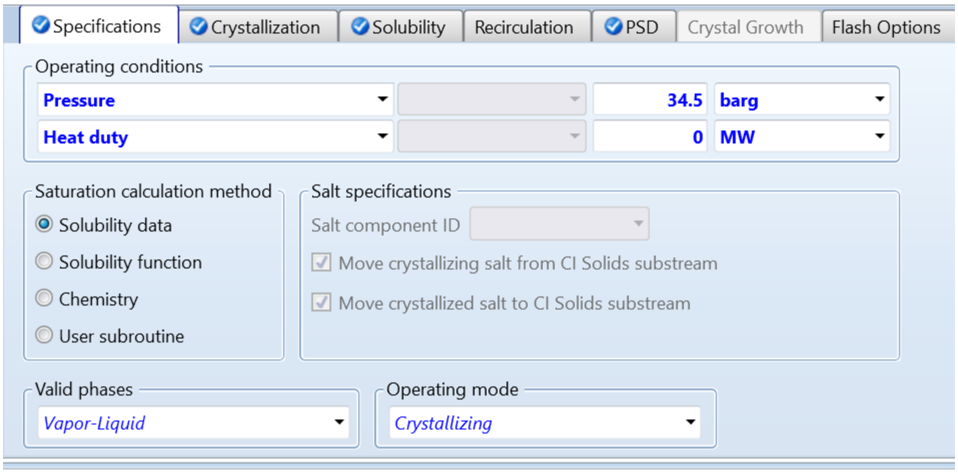
Reactor dimensions

Length 7.4 meter

Diameter 2.8 meter

Figure 19: Reactor Results in Aspen Plus Simulation

6.2.6 C-101 Specification



Operating conditions

Pressure		34.5	barg
Heat duty		0	MW

Saturation calculation method

● Solubility data
○ Solubility function
○ Chemistry
○ User subroutine

Salt specifications

Salt component ID

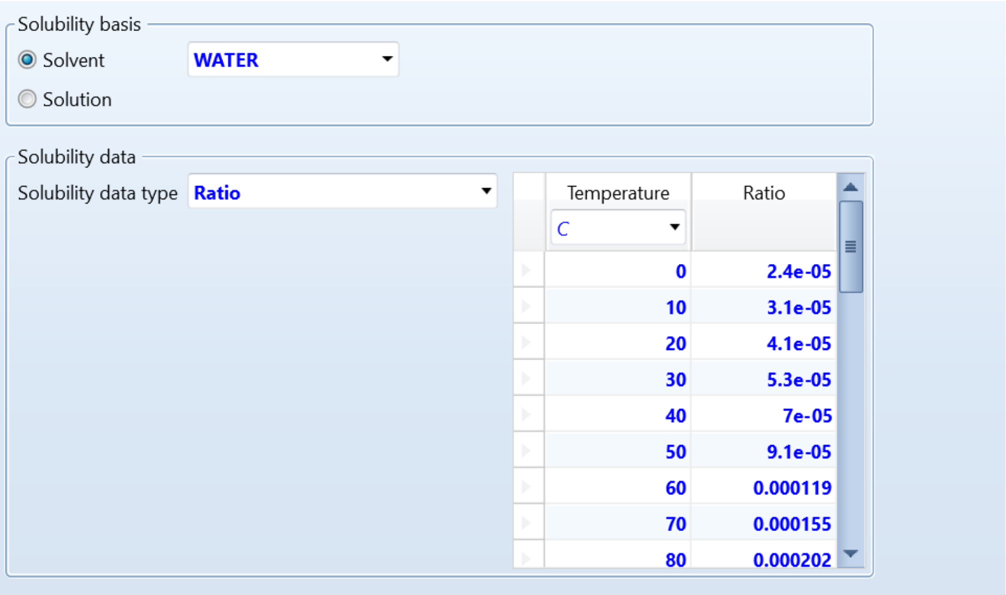
☑ Move crystallizing salt from CI Solids substream
☑ Move crystallized salt to CI Solids substream

Valid phases: *Vapor-Liquid*

Operating mode: *Crystallizing*

Figure 20: C-101 Specifications

6.2.7 C-101 Solubility Data



Solubility basis

● Solvent WATER
○ Solution

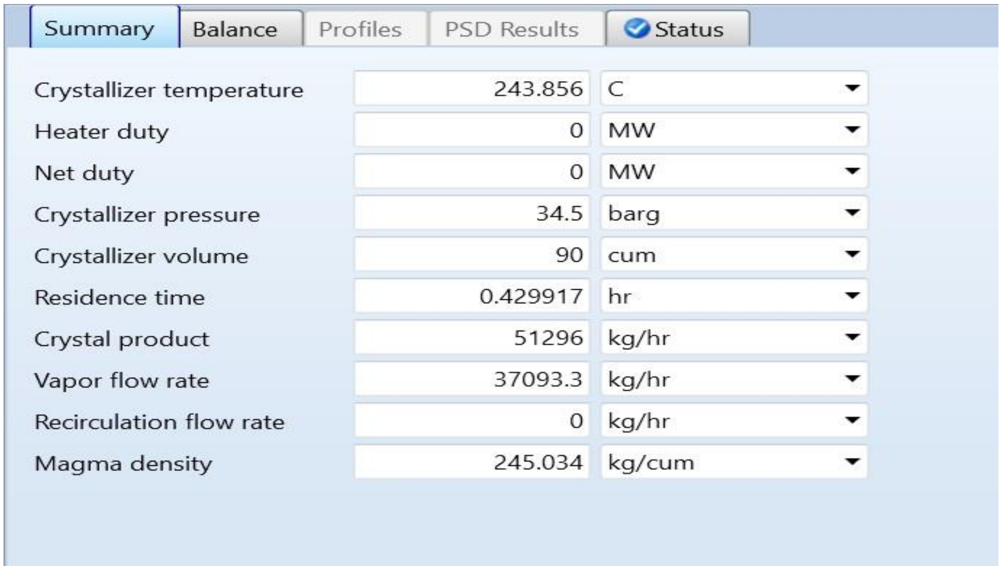
Solubility data

Solubility data type: Ratio

Temperature	Ratio
C	
0	2.4e-05
10	3.1e-05
20	4.1e-05
30	5.3e-05
40	7e-05
50	9.1e-05
60	0.000119
70	0.000155
80	0.000202

Figure 21: C-101 Solubility Data

6.2.8 C-101 Results



Crystallizer temperature	243.856	C
Heater duty	0	MW
Net duty	0	MW
Crystallizer pressure	34.5	barg
Crystallizer volume	90	cum
Residence time	0.429917	hr
Crystal product	51296	kg/hr
Vapor flow rate	37093.3	kg/hr
Recirculation flow rate	0	kg/hr
Magma density	245.034	kg/cum

Figure 22: C-101 Design Results

CHAPTER 7

INSTRUMENTATION

7.1 Instrumentation Overview:

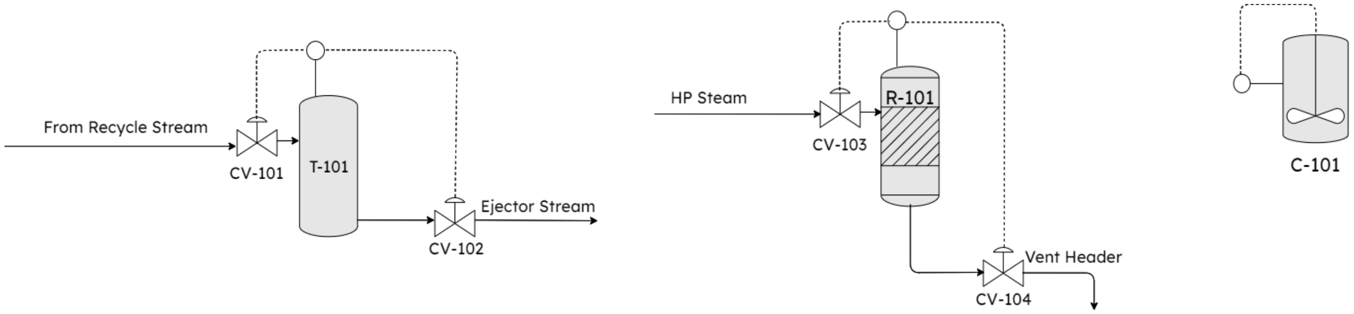


Figure 23: Instrumentation Overview

7.1.1 Instrumentation - Level Control:

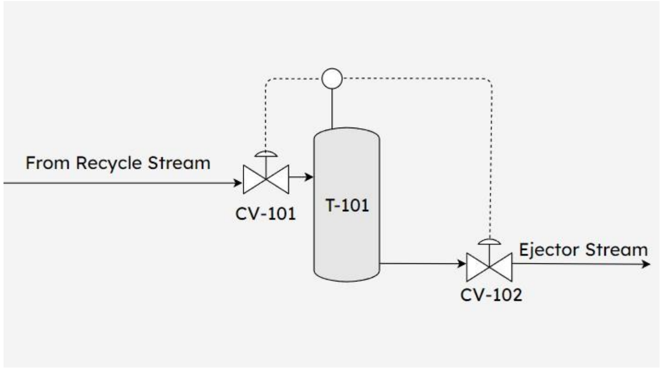


Figure 24: Instrumentation – Level Control

- Install a Level Control sensor (shown in diagram)
- The Sensor is connected to LCV-101 and LCV-102 control Valves to maintain the level of the tank
- Maintaining a consistent level in the feed tank ensures a steady supply of slurry to downstream processes.

7.1.2 Instrumentation - Pressure Control:

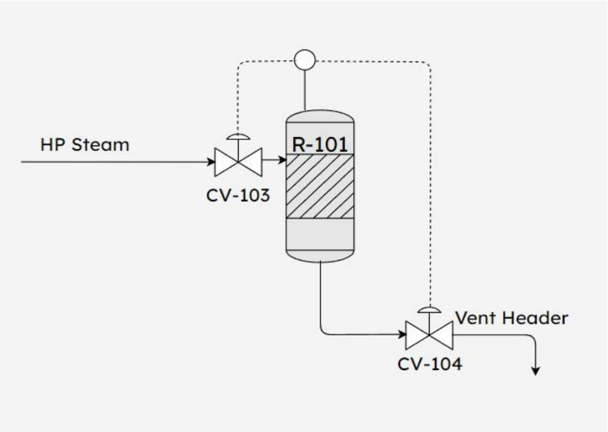


Figure 25: Instrumentation – Pressure Control

- Install a Pressure Control sensor (shown in diagram)
- The Sensor is connected to PCV-103 and PCV-104 control Valves to maintain pressure through the introduction of HP steam or venting steam incase of higher pressures
- Pressure sensor data can be logged and analyzed over time to be used for process optimization and predictive maintenance

7.1.3 Instrumentation – Temperature:

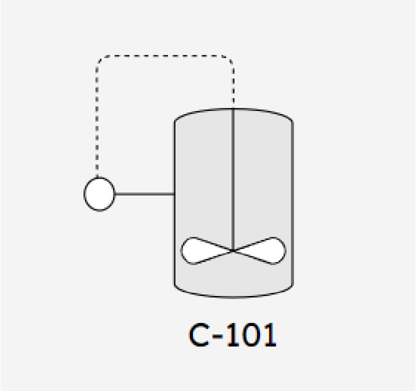


Figure 26: Instrumentation – Temperature

- Install a Temperature Control sensor (shown in diagram)
- The Sensor is connected to an agitator housed withing the Crystallizer
- Connecting a temperature sensor to an agitator in a crystallizer facilitates more efficient heat distribution and transfer, promotes uniform crystal growth, and allows for precise control over the cooling or heating rates

CHAPTER 8

ECONOMIC ANALYSIS

8.1 : Introduction

Cost estimation is a critical aspect of chemical engineering design. It allows engineers to evaluate the economic viability of a project by determining the necessary capital investment and production costs. There are three main types of cost estimations:

Preliminary estimates: These are rough estimations used in the early stages of a project to assess feasibility and compare design alternatives. They typically have an accuracy of around 30%.

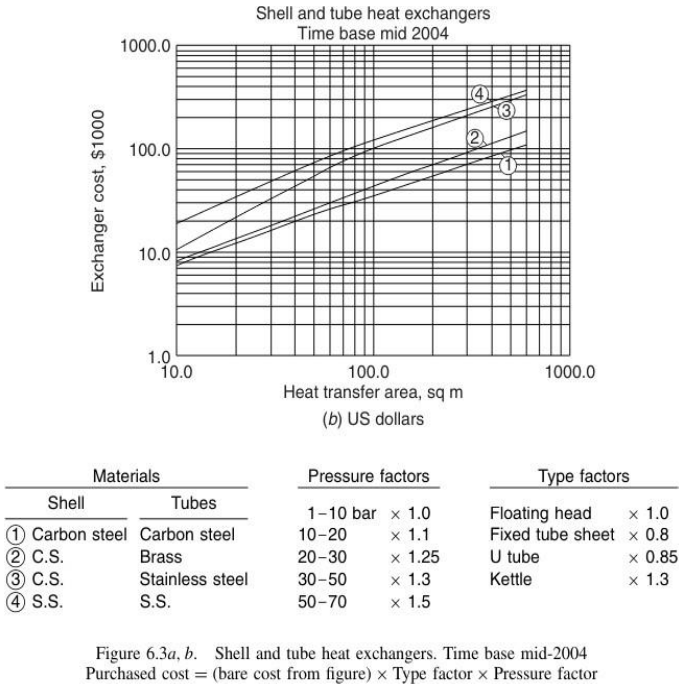
Authorization estimates: These are more detailed estimations used for budgeting and project authorization. They typically have an accuracy of 10-15%.

Detailed estimates: These are the most accurate estimations, used for project cost control and fixed price contracts. They are based on the final design and firm equipment quotes, and typically have an accuracy of 5-10%.

The cost of preparing an estimate increases with the desired level of accuracy. The factorial method is a common approach to cost estimation, where the cost of each piece of equipment is estimated based on its specifications and relevant factors.

Table 24: E-103 Specifications

For E-103	
Heat Transfer Area (m^2)	161.4
Materials	Stainless Steel
Pressure Factor	1.6
Type Factor	0.8
Cost ($)	366,592



Materials	
Shell	Tubes
① Carbon steel	Carbon steel
② C.S.	Brass
③ C.S.	Stainless steel
④ S.S.	S.S.

Pressure factors	
1–10 bar	× 1.0
10–20	× 1.1
20–30	× 1.25
30–50	× 1.3
50–70	× 1.5

Type factors	
Floating head	× 1.0
Fixed tube sheet	× 0.8
U tube	× 0.85
Kettle	× 1.3

Figure 6.3*a*, *b*. Shell and tube heat exchangers. Time base mid-2004
Purchased cost = (bare cost from figure) × Type factor × Pressure factor

Figure 27: Exchanger Cost

8.2 : Main Equipment's Cost

Table 25: Main Equipment Cost

Specification	Equipment Cost ($)
Feed Tank	208,435
Reactor	195,468
Heat Exchangers	1,768,806
Crystallizers	214,200
Centrifuge	56,000
Dryer	98,643
Total	2,541,552

8.3 : Total Investment

Table 26: Total Investment

PCE (after adjusting for Inflation) $ 2,541,552.16	
f1 (Equipment erection)	0.4
f2 (Piping)	0.7
f3 (Instrumentation)	0.2
f4 (Electrical)	0.1
f5 (Buildings, process)	0.15
*f6 (Utilities)	-
*f7 (Storages)	0.15
*f8 (Site development)	-
*f9 (Ancillary buildings)	-
f10 (Design and Engg.)	0.3
f11 (Contractor's fee)	0.05
f12 (Contingency)	0.1
(Total Physical Plant Cost) PPC = PCE (1+f1+…….+f9)	$6.86M
(Fixed Capital) FC = PPC(1+f10+f11+f12)	$9.95M
Working Capital (15% of FC)	$1.49M
Total Investment Required (Fixed Capital + Working Capital)	$11.4M
Operating Time of Plant	347 days/year

8.4 : Direct Production Cost

Table 27: Fixed Operating Cost

Fixed Operating Cost		
Maintenance (3-5% of FC)	$	497,509
Operating Labor (OL)	$	60,000
Plant Overheads (50% of OL)	$	30,000
Laboratory (30% of OL)	$	18,000
Capital Charges (4% of FC)	$	398,007
Insurance (1% of FC)	$	99,502
Local Taxes (2% of FC)	$	199,004
Total Fixed Operating Cost	$	**1,302,021**

Table 28: Variable Operating Cost

Variable Operating Cost	
CTA Feed Rate	***1098.6 ton/day***
CTA Feed Price	$ 945/ton
CTA Feed Cost	$ 1,038,211.9/day
CTA Feed Cost	$ 360,259,553.7/yr
Water Requirement	***2563.5 ton/day***
Water Price	$ 1/ton
Water Cost	$ 935,671.7/yr
Catalyst (Pd/C) Quantity Required	***21,612.5 kg/yr***
Catalyst (Pd/C) Price	$ 100/kg
Catalyst (Pd/C) Cost	$ 2,161,250/yr
Steam Quantity Required	***165,692.8 ton/yr***
Steam Price	$ 280/ton
Steam Cost	$ 46,393,988.8/yr
H_2 cost	$ 1200/yr
Miscellaneous Operating Material (5% of Maintenance Cost)	***$ 24,875.4***
Electric Power	1,124,280 MJ/yr
Price of electricity	$ 0.027/MJ
Cost of electricity	$ 30,355.56/yr
Total Variable Cost (TVC)	$ **409,806,894.6**

Direct Production Cost (TFOC+TVC)	$ 411.1M
Indirect Production Cost (20% of Direct Cost)	$ 82.2M
Annual Operating Cost	$ 493.3M

8.5 : Revenue Generated

Revenue			
Product	Production (ton/yr)	Price ($/ton)	Revenue Generated ($)
Pure Terephthalic Acid	400,000	1,250	500M
		Total Revenue/yr	**500M**
		Total Profit/yr	**6.66M**

Table 29: Revenue Generated

8.6 : Payback Period

Table 30: Payback Period (1)

Payback Period				
No. of Years (k)	Cash Inflow ($)	Cash Outflow ($)	Net Cash Flow ($)	Net Present Worth ($) (22%)
0	-	11.4M	-11.4M	-
1	500M	493.3M	6.66M	5.46M
2	500M	493.3M	6.66M	4.48M
3	500M	493.3M	6.66M	3.67M
4	500M	493.3M	6.66M	3.01M
5	500M	493.3M	6.66M	2.46M

Table 31: Payback Period (2)

No. of Years (k)	Cumulative Present Worth ($)
0	- 11.4M
1	- 5.97M
2	- 1.49M
3	2.17M
4	5.18M
5	7.65M
Payback Period	**2.9 Years**

CHAPTER 9

HAZOP ANALYSIS

9.1 : HAZOP Methodology

HAZOP, which stands for Hazard and Operability Study, is a structured and systematic method used to identify and evaluate potential hazards and operability problems in a process plant or system. It is primarily used during the design or modification phase of a process to ensure that hazards are identified and that adequate safeguards are put in place to prevent accidents.

The HAZOP methodology involves a multidisciplinary team of experts who systematically analyze the process by breaking it down into smaller sections called nodes. Each node represents a specific piece of equipment, a process step, or an operating instruction. The team then considers various process parameters, such as flow, temperature, pressure, and composition, and applies guide words like "No," "More," "Less," "Reverse," "Other Than," and "Part of" to these parameters to identify potential deviations from the intended design or operating conditions.

For each deviation, the team brainstorms possible causes and consequences. The causes could be equipment failures, human errors, or external events. The consequences could range from minor operational issues to major accidents with significant safety, environmental, or economic impacts. The team also identifies existing safeguards, such as alarms, interlocks, or relief systems that could mitigate the identified hazards.

9.2 : HAZOP Analysis on Reactor

Table 32: Reactor Flow HAZOP

Item	Study node	Process parameters	Deviations (Guide words)	Possible Causes	Possible Consequences	Action Required
1A	Reactor	Flow	No	Failure of hydrogen supply valve	Incomplete reaction, reduced production	Check and repair/replace the hydrogen supply valve, implement redundant valves or backup systems, and implement an alarm system
				CTA supply failure	No reaction, loss of production	Investigate and address the CTA supply failure, check for blockages or leaks, and implement redundant CTA supply systems
1B			High	Malfunction of hydrogen flow control valve	Over pressurization, increased reaction rate	Repair or replace the malfunctioning hydrogen flow control valve, install pressure relief valves or safety valves, and implement an alarm system
				Malfunction of steam flow control valve	Excessive heat transfer, potential reactor overheating	Repair or replace the malfunctioning steam flow control valve, install additional temperature sensors, implement automated systems, and ensure proper insulation and cooling mechanisms

1C			Low	Steam supply failure	Inadequate heat transfer, reduced reaction rate	Investigate and address the steam supply failure, check for blockages or leaks, and implement redundancy in the steam supply system
1D			Reverse	Backflow due to incorrect valve positions	Disruption of heat transfer, potential reactor overheating	Correct valve positions, install check valves or non-return valves, and implement regular inspections and maintenance
1E			Sooner	Premature opening of hydrogen supply valve	Uncontrolled reaction, increased reaction rate	Implement interlocks or safety systems, improve control system response time, and enhance operator training and awareness
1F			Later	Delayed opening of CTA supply valve	Inadequate reaction time, reduced production	Improve response time of the CTA supply valve, monitor and optimize CTA feed scheduling, and implement backup systems

Table 33: Reactor Pressure HAZOP

Item	Study node	Process parameters	Deviations (Guide words)	Possible Causes	Possible Consequences	Action Required
1A	**Reactor**	**Pressure**				
			More/Higher	Malfunction of pressure control valve or excessive steam flow	Over pressurization, potential reactor failure	Repair or replace the malfunctioning pressure control valve, install pressure relief valves or safety valves, and implement an alarm system to monitor and control pressure levels
1B			Less/Lower	Insufficient steam supply or pressure drop	Inadequate heat transfer, reduced reaction rate	Investigate and address the steam supply failure, check for blockages or leaks, and ensure sufficient steam pressure is maintained
1C			Sooner	Premature increase in pressure due to rapid heating	Uncontrolled reaction, potential safety hazards	Implement interlocks or safety systems to prevent rapid heating, improve control system response time, and enhance operator training and awareness
1D			Later	Delayed increase in pressure	Inadequate reaction time,	Optimize heating processes, monitor and adjust heating

				due to slow heating	reduced production	rates, and ensure proper heat transfer mechanisms are in place

Table 34: Reactor Temperature HAZOP

Item	Study node	Process parameters	Deviations (Guide words)	Possible Causes	Possible Consequences	Action Required
	Reactor	Temperature				
1A			Higher	Malfunction of temperature control system or excessive heating	Overheating, potential reactor failure	Repair or replace the malfunctioning temperature control system, install additional temperature sensors, implement automated systems for temperature control, and ensure proper insulation and cooling
1B 1C			Lower	Insufficient heating or cooling system performance	Inadequate heat transfer, reduced reaction rate	Investigate and address the heating or cooling system failure, check for blockages, leaks or malfunctioning components, and ensure proper calibration and maintenance of the temperature control equipment
1D			Sooner	Rapid increase in temperature due to process anomalies or control failure	Uncontrolled reaction, potential safety hazards	Implement interlocks or safety systems to prevent rapid temperature rise, improve control system response time, and enhance operator training and awareness

CONCLUSION

We have enhanced the output of Purified Terephthalic Acid and decreased wastage of the unusable extra Crude Terephthalic Acid.

By extending the purification facility to process the additional 1100 tons of CTA per day. With a low initial total investment, this has resulted in additional revenue of $500 million.

The new purification plant was built to be more efficient than the old one, which contributed not just to the increase in PTA production but also to the overall increase in production. Better quality control: the newly constructed purification plant was outfitted with cutting-edge machinery that contributed to an improvement in the product's overall quality, which in this case was the PTA. Because of this, there was a subsequent rise in demand for the PTA goods offered by the company.

The increased production of PTA has brought about a variety of positive outcomes for the corporation, including the following:

As a direct result of the increased PTA production, the company has seen an increase in revenue of $13 million as a direct result of the higher output.

Profitability has increased as a result of the increased income and the decreased costs that are linked with the new purification facility. This has led to an improvement in the profitability of the business.

Enhanced market position: the firm's market position has been enhanced as a result of the increased production of PTA as well as the improvement in the quality of the PTA products that the company manufactures.

The corporation made a smart investment by expanding its facility that handles the purification process. As a direct consequence, we have seen a rise in sales, an improvement in profitability, and an improvement in our position in the market. Because of this investment, the company now has a solid foundation upon which to build its future expansion.

In addition to the benefits that were discussed previously, the enlargement of the plant that performs the purifying process has also assisted in cutting down on the amount of unused CTA that is created whenever there is a surplus. This is due to the fact that the newly constructed purification facility is more effective than its predecessor in terms of both efficiency and quality control. As a consequence of this, the business is in a position to generate a greater quantity of PTA from each ton of CTA that it employs. Both the company's financial situation and its impact on the surrounding environment have improved as a result of these change

RECOMMENDATIONS FOR FUTURE RESEARCH

- In the interest of enhancing PTA output, additional study may be directed on the optimization of the crystallization process. To achieve this goal, it may be necessary to investigate various process parameters, such as temperature, pressure, residence time, and cooling rates, in order to improve crystallization productivity and yield.

- Development of a Comprehensive Kinetic Model for the Crystallization Process: The development of a comprehensive kinetic model for the crystallization process can provide useful insights into the underlying mechanisms and assist in the process of improving the process. In subsequent investigations, the formulation and verification of mathematical models may play a role in elucidating the nucleation, growth, and agglomeration behaviors that occur throughout the crystallization process.

- Elimination of Impurities: The synthesis of PTA from CTA necessitates the elimination of impurities in order to reach the appropriate levels of purity. In the future, research may investigate more advanced methods of purification, such as adsorption, filtering, or membrane processes, with the goals of improving the effectiveness of impurity removal and reducing the overall expenses of the process.

- Process Monitoring and Control: The development of innovative monitoring and control systems has the potential to improve the crystallization process's operational efficiency as well as its dependability. In the future, research can investigate the possibility of integrating advanced control algorithms with real-time process monitoring technologies, such as spectroscopy or imaging methods, in order to enable better process control and optimization.

- Energy Efficiency: Investigating energy-efficient methods for the crystallization process can be beneficial to both the environment and the bottom line.

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