

## PRODUCTION OF PARA-XYLENE VIA ISOMERIZATION

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**ABSTRACT:** Energy recently, there has been an increase in use of xylene in industrial, domestic and agriculture sector. Xylene is an aromatic hydrocarbon and has three isomers named paraxylene, orthoxylene and meta xylene. All these isomers are extensively use in different industries. Due to increase in use of xylene there has been huge demand for the production of xylene. Which creates a challenge for industrial sector scope the demand. The research focus explains the production of xylene using catalyst to meet the world demand. The recovery process involves a two stage crystallization process with multiple reflux streams meant to increase the yield of the para-xylene recovery such that the product of the crystallization process is a 99% pure stream in para-xylene. The second process involving production of para-xylene via isomerization over a ZSM-5 catalyst is fed with the stream rich in meta-xylene from the crystallization process. This research also focus on the material, energy balance and simulation results are included for the production of para-xylene.

**Keywords:** Para-xylene; Xylene; Ethyl benzene; Crystallization; Isomerization.

### 1. INTRODUCTION

Xylene is a colorless fluid with a sweet scent occurring basically in oil and coal tar. Though, xylene is principally a manmade chemical and is mostly delivered from petroleum. There are three isomers of xylene having a similar chemical formula, however with various configurations. For the production of xylene, a blend of the three isomers is generally framed and different synthetic substances may present on the littler amount, for example, benzene and ethylbenzene [1].

Para-xylene is one of the three isomers of xylene. Para-xylene is a fragrant hydrocarbon dependent on benzene with two substituents with the s chemical formula  $C_8H_{10}$  or  $C_6H_4(CH_3)_2$ . The "p" represents para, distinguishing the area of the methyl bunches as opposite each other. Other xylene isomers include ortho-xylene and meta-xylene. Para-xylene is produced by catalytic reforming of petroleum naphtha as a part of the BTX (benzene, toluene, and xylenes) aromatics extracted from the catalytic reformat. The para-xylene is then separated in a series of distillation, absorption or crystallization and reaction processes from the meta-xylene, ortho-xylene and ethylbenzene. Other xylene isomers incorporate ortho-xylene and meta-xylene. Para-xylene is made by catalytic transforming of oil naphtha as a piece of the BTX (toluene, benzene and xylenes) aromatics separated from the catalytic reformat. The para-xylene is then isolated out in a progression of refining, reaction processes and absorption or crystallization from the meta-xylene, ortho-xylene and ethylbenzene [1, 2].

Para-xylene weighing  $106.17 \text{ g.mol}^{-1}$  appears as either colorless fluid or colorless crystalline solids with a fragrant smell. The scent limit of para-xylene is 0.62 ppm. The breaking point of para-xylene is  $138.3 \text{ }^\circ\text{C}$  ( $281 \text{ }^\circ\text{F}$ ) and the softening point is  $13.2 \text{ }^\circ\text{C}$ . The colorless fluid is insoluble in water and is profoundly dissolvable in ethanol and diethyl ether. Para-xylene has a specific gravity of 0.86 and it's combustible having a glimmer purpose of  $27 \text{ }^\circ\text{C}$  or lower. Vapor pressure and viscosity noted at  $20 \text{ }^\circ\text{C}$  is  $9 \text{ mmHg}$  and  $0.6475 \text{ cP}$  respectively. Figure 1 shows the raw materials and product of para-xylene [3].

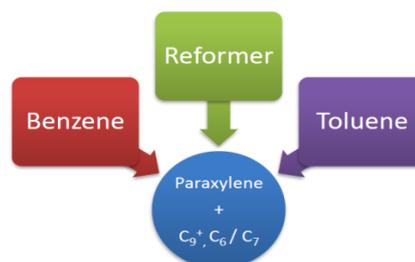


Fig. 1. Raw material and product of para-xylene

Xylene are in demand as solvents and thinners for varnishes and paint. They are also used in aircraft fuel and gasoline besides having a moderate market in leather, cleaning agents and rubber industry. However, para-xylene amongst the three isomers is in large demands since it forms the major raw material for the production of terephthalic acid (TPA) which later converts to dimethyl-terephthalate (DMT). DMT is then responded with ethylene-glycol to frame polyethylene-terephthalate (PET). PET is the crude material for most polyester utilized in the production of fibers, bundling materials, PET containers and bottles. Small amounts of para-xylene are also used in the production of diparaxylene for herbicides [2, 4].

Worldwide interest for para-xylene has been developing insistently and this is required to proceed. The world utilization has developed at a normal of 7 percent per year in the 2013-2018 period. Development in Asia was higher at a normal of 8.5 percent per year in a similar period, driven by China. The global market for para-xylene is driven by the significant growth observed across the global polyester market in the past few years, which is led by the rising demand from textile applications, and the high demand for polyethylene terephthalate (PET) in the Asia Pacific. Although the market is expected to embark upon a smooth growth path in the region in the next few years, it will witness limited growth avenues in developed regions such as North America and Europe. Strict government regulations regarding the proper use of non-biodegradable materials and rising consumer awareness about the use of plastic-free products will have the most drastic influence on the consumption of para-xylene across these regions [1, 3].

Demand for para-xylene is the largest when compared to other xylene isomers due to its end product market, its demand was rising at an annual rate of 3.2% between 1998 and 2018, and increased from 7.1 billion lb to 13.4 billion lb. Nevertheless, the global para-xylene market will continue to exhibit growth at a healthy pace owing to demand across the textile and packaging industry and expand at a 7.0% CAGR ended the period among 2016 to 2024. If the number holds true, the market, which had a valuation of US\$ 33.03 in 2015, will reach US\$ 60.04 by 2024 [1, 3].

In America, para-xylene is solely used for the production of PET which has the largest consumption in the USA than anywhere else in the world. Considering the never-ending domestic demand America has planned its melt phase para-xylene production capacity to avoid bottlenecks in its production operations in the near future. Para-xylene, which serves as the important chemical, has delighted in a broad application in numerous fields of chemical production in China [5].

To develop an understanding of the production of para-xylene via isomerization and recovery using the crystallization technique from a feed of mixed xylene and ethyl benzene. The production of large amounts of heavy naphtha is inevitable in refineries across Pakistan. Failure to extract key components from it and heavy reliance on the import of those components is the motivation behind the work for this research. Amongst other components which are also of immense importance para-xylene holds extraordinary importance for Pakistan in virtue of its market both domestic and international. This research is based on the production and recovery of para-xylene with pre-coked ZSM-5 catalyst.

### 1.1. Recovery and Production of Para-Xylene

Modernly the greater part of the para-xylene is delivered by catalytic improving of naphtha. The catalytic changing of naphtha brings about the creation of xylene isomers and different aromatics. Aside from the catalytic changing different techniques incorporate the transformation of toluene, for example, the unbalanced and methylation with methanol of toluene. Toluene has the least interest when contrasted with benzene and xylenes and there is a solid motivating force to change over surplus toluene to progressively significant aromatics. Figure 2 demonstrates the correlation of overall BTX dispersion examples of production and market request. The interest for toluene is just 11% of the all-out BTX and it very well may be changed over to progressively significant aromatics like para-xylene [6, 7].

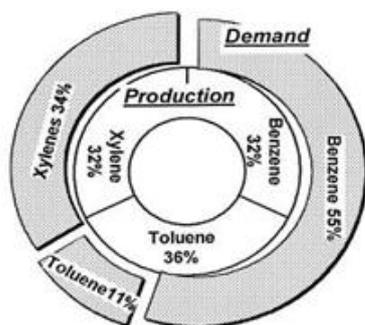


Fig. 2. Comparison of worldwide BTX distribution of production and market demand.

Nowadays the key source of the making of para-xylene and different aromatics, BTX, is reactant improving naphtha

and somewhat the results of the steam breaking of naphtha. In any case, these techniques produce a dilute mixture of para-xylene with other insignificant isomers, meta-xylene and ortho-xylene, alongside ethyl benzene. Table 1 indicates naphtha circulation and overall interest of xylene isomers [7].

Table 1. Worldwide demand for feedstock distribution of xylene isomers

Xylene Isomers	Ethyl-Benzene	Para-xylene	Meta-xylene	Ortho-xylene
	Distribution			
Reformed Naphtha	18%	21%	41%	20%
Pygas (C <sub>8</sub> ) cut	52%	12%	25%	11%
Demand for separated isomers	1%	86%	3%	10%

Because of the inadequacies of these techniques to create para-xylene of the required purity, filtration is done to isolate para-xylene from these compounds, which have close boiling points. To expand the volume of p-xylene created isomerization is completed to change over meta-xylene into para-xylene and ortho-xylene.

BTX aromatics created by catalytic improving are isolated from non-fragrant raffinate using extraction. Further detachment of the BTX aromatics is done to get benzene, toluene and C8 xylene streams in the product recuperation area. Para-xylene is typically recuperated by either crystallization technique or adsorption strategy [8].

Catalytic methylation of toluene is a potential choice to create para-xylene if the expense of methanol stays low. By responding toluene and methanol over a zeolite catalytic, for example, ZSM-5, water and xylenes are shaped with the accompanying equilibrium composition of xylene isomers; 23.55% para-xylene, 52.42% meta-xylene and remaining ortho-xylene at 750 °F [7, 8].

The process of isomerization of meta-xylene is a catalytic reaction over a zeolite-based catalyst; the reaction is a reversible one with high reaction rate constant for the forward reaction when compared to the reversible reaction of isomerization of para-xylene. Isomerization of meta-xylene involves two parallel reactions, otherwise known as the methyl shift reaction. Converting meta-xylene into para-xylene and ortho-xylene, a para-xylene selective catalyst modification is essential for increasing the yield of para-xylene production [9].

### 1.2. Methods available for recovery

The boiling points of the diverse xylene isomers are exceptionally near one another, this represents a test in the partition of para-xylene from mixed xylene and requires broad vitality to be completed. The modern techniques use for xylene separation are discussed. These techniques are contrasted in the capital and operating expense.

Because of extremely close boiling points of xylenes, it is a test to isolate para-xylene from its isomers. To isolate ortho-xylene and meta-xylene we should do broad refining. Isolating meta-xylene and para-xylene utilizing the refining procedure isn't financially suitable. Because of the wide scope of freezing points, as appeared in Table 2, it is conceivable to isolate xylene isomers by bringing down the temperature. Para-xylene will take shape first as it has the most elevated the freezing points and the solid crystals can be isolated by utilizing any physical partition procedures like filtration and centrifugation [7].

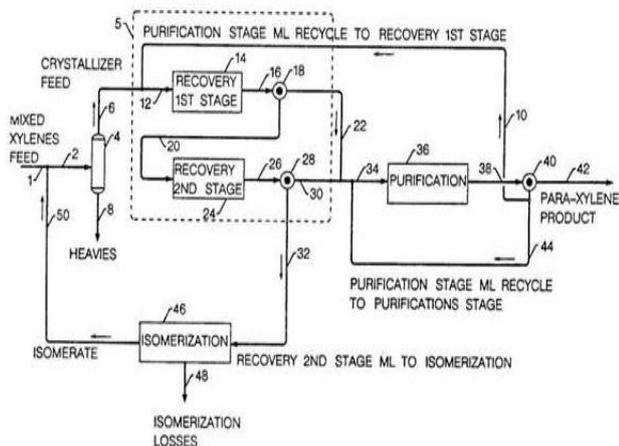
**Table 2. Physical properties of xylene isomers**

Compound	Normal boiling Point °C	Freezing Point °C
Benzene	80.1	5.5
Toluene	110.6	-95.0
Para-xylene	138.3	13.2
Meta-xylene	139.1	-47.9
Ortho-xylene	144.3	25.3

Para-xylene and meta-xylene can be separated by reactive purification. This process comprises alkylation the mixture of xylenes. Meta-xylene reacts especially with Di-Tertiary Butyl-Benzene (DTBB and normal boiling point 230 °C) and Tertiary Butyl-Benzene (TBB and normal boiling point 169.3 °C) to form Tertiary Butyl Meta-Xylene (TBMX and normal boiling point 205 °C) and benzene. Meta-xylene forms Tertiary Butyl Meta-Xylene which boils at a higher temperature and can be separated easily from para-xylene [7, 10].

## 2. METHODOLOGY

The process to be studied is divided into two parts for simplicity namely recovery of p-xylene and its production via the isomerization reaction.



**Fig. 3. BFD for the combined process of recovery and production of para-xylene.**

The process of para-xylene production and recovery is a complex overall train since the two minor processes work in conjunction. Figure 3 displays the simplified block flow diagram of the two processes. The scope of this particular process is to increase the purity and yield of the desired product that is para-xylene. Feed to the process is a mixture of xylenes and ethylbenzene which is introduced in a recovery section denoted by the dotted box in Figure 3. The recovery process involves a two-stage crystallization process with multiple reflux streams meant to increase the yield of the para-xylene recovery such that the product of the crystallization process is a 99% pure stream in para-xylene. The second process involving the production of para-xylene via isomerization over a ZSM-5 catalyst is fed with the stream rich in meta-xylene from the crystallization process. The waste of this reaction may further be separated to extract aromatics compound of high demand through various separation techniques, these compounds may include ethylbenzene, benzene, toluene and higher aromatics [7, 11].

### 2.1. Recovery by crystallization

A moisture-free mixed xylene feed *stream 1* having 56.77% meta-xylene, 25.1% para-xylene, 10.24% ortho-xylene and 7.29% Ethyl Benzene by weight leave the drier at 105 °F and 75 psig. This stream enters the feed chiller before being fed into the first of two-stage parallel crystallizer arrangement [12].

Cooled xylene feed stream 2 leaves the chiller at -10 °F and is split evenly into two streams. These split stream, streams 3 are entering the first stage crystallizers parallel arrangement for increased recovery of para-xylene overall at -10 °F, where the first stage nucleation of para-xylene crystals takes place. The mother liquor is further cooled to a temperature of -45 °F at 1psig in a scraped surface crystallizer which is assumed as a simple shell and tube heat exchanger of duty 500,000Btu/hr.

It is assumed that small crystal formation is initiated in the first of the two crystallizers arranged in series. Streams 4 leave the second crystallizers at -79 °F and 30 psig and enter the centrifuge. Ethylene is used as the first stage crystallizer chilling agent. Ethylene is fed to the first stage first crystallizer at a temperature of -71 °F and at a temperature of -105 °F to the first stage second crystallizer. In the centrifuges, the newly formed para-xylene crystals are separated from the mother liquor. The streams that exit the centrifuges streams 5 leave at a temperature of 100 °F and a pressure of 3 psig and enter the melt tank, this stream is 20% of the feed to the centrifuges. Also leaving the centrifuges are streams 6 that are 80% of the centrifuge feed, at the same conditions for pressure and temperature, which are fed to surge drum. This is to ascertain that sufficient room is left in the centrifuge to ensure maximum efficiency.

Stream 6a leaves the surge drum being maintained at a temperature of -59 °F and is fed back into the centrifuges as to favor increased efficiency of the centrifuge. 80% of stream 6 is stream 6b that is rich in meta-xylene content leaves the surge drum and is fed into the chiller to exchange heat to lower the temperature such that to reduce the duty of the first stage crystallizers.

Stream 7 leaving the melt tank is immediately split into three streams; stream 7a, stream 7b and stream 7c. Stream 7a is an 80% recycle stream of the discharge of the melt tank is fed back into the melt tank at a temperature of 150 °F and pressure of 35 psig after being passed through a heater of duty 1185000 Btu/hr. Stream 7b at conditions of 64 °F and 35 psig carries the relatively rich para-xylene feed for the second stage crystallization process, this stream then splits into two equivalent streams 7c which is the feed for the second stage parallel crystallizers.

The feed to the second stage crystallization is now containing 85% by wt. para-xylene. Second phase of the crystallization occurs here in a parallel combination of crystallizers as shown in Figure 3. Since the feed to the crystallizer is rich in para-xylene the temperature of the crystallizer is now maintained at 25 °F approximately close to the melting point temperature of 55 °F of para-xylene. The second stage crystallizers are designed at a duty of 417000 Btu/hr. The reduced duty of the second stage crystallizer has allowed for the second choice of refrigerant that is Propane which is fed into the crystallizer at a temperature of -1 °F.

Streams 8 leaving the second stage crystallizers at 25 °F and 30 psig. Streams 8 merge and form stream 8a which is fed into the centrifuge at the same conditions for temperature and pressure as the streams 8. Leaving the centrifuge are two streams; stream 9 and stream 10. Stream 9 is fed into the recycle surge tank, whereas stream 10 is fed into the melt tank at 100 °F and 3 psig similar to the first stage melt tank. Stream 11 leaves the melt tank at 100 °F and 35 psig and is split into two streams; stream 12 and

stream 13. Stream 12 passes through a heater is heated to a temperature of 150 °F with a very small pressure drop the pressure is assumed to remain the same, 35 psig. This stream is recycled into the centrifuge to increase the efficiency of the centrifuge.

Stream 13 is directed to the para-xylene test tank from where it runs down to the p-xylene storage tank for marketing. Stream 14 leaves the recycle surge tank and splits into streams 15a and 15b. Stream 15a is recycled into the centrifuge which is 92% of stream 14 whereas stream 15b splits into two further streams; stream 16 which is a 75% recycle stream to second stage crystallizer feed while the remaining 25% of stream 15b which is recycled and becomes stream 17 in the first stage crystallizer feed stream 2. Stream 16 is a para-xylene rich stream and merges into stream 7b to increase the yield of para-xylene.

## 2.2. The production process of para-xylene via Isomerization

The xylene feed from the tank stream 1 at 113 °F and atmospheric pressure is passed through the octafiner charge which increases the pressure of this stream to 280 Psig. After passing through the octafiner charge stream 1 is joined by recycle stream that is stream 2 which is a mixture of vapor from the flash drum and some fresh gas that is coming from the H<sub>2</sub> purifier. Stream 2 has a temperature of 185 °F. Stream 1 and 2 join together to make stream 3 and stream 3 is at 155 °F and 217 psig, which is passed through a heat exchanger and the temperature increases to 875 °F this is to lower the duty of the furnace that follows [13].

This stream is fed into the furnace for heating to a temperature of 950 °F. Stream 3 then leaves the furnace after being heated up to a temperature of 950 °F and enters the reactor where the isomerization reaction takes place. Stream 4 is the reactor effluent which leaves the reactor at 952 °F and a pressure of 173.5 psig. Stream 4 passes through the feed effluent exchanger and loses a majority of its heat content while exchanging the heat with the fresh feed stream. When it exits the exchanger its temperature has dropped to 210 °F. Then it is further cooled by an air effluent condenser where its temperature drops to 135 °F. However stream 4 needs to be cooled some more before it can be allowed to enter the flash drum, so it is passed through another effluent condenser or trim cooler which drops the temperature down to about 100 °F.

Two streams leave the flash drum, stream 5 and stream 6. Stream 5 is the feed to the light aromatics column and it enters the column at a temperature of 268 °F after having passed through an exchanger that increases its temperature. Stream 6, however, is the flash drum vapor and is split into two streams, one stream is used as fuel gas, whereas the other is recycled and joins the fresh gas feed which makes stream 2.

Three streams leave the light aromatics column. They are stream 7, stream 7a and stream 8. Stream 7 is the light aromatics column bottom product and leaves the column at a temperature of 322 °F it is passed through an exchanger to heat stream 5 whereby getting cooled to 145 F itself and then further cooled to 110 °F by being passed through a cooler. The stream is then fed to the o-xylene charge tank. Stream 7a leaves the bottom of the light aromatics column

and is fed to the re-boiler before being recycled into the light aromatics column. Stream 8 leaves the top of the aromatics column at 250 °F. It is cooled down to 145 oF by an air-cooled condenser and then if further cooling is required by the trim cooler to a temperature of 100 °F. Then it enters an accumulator drum and is split into two streams, stream 8a and stream 8b. Stream 8a leaves the drum and is called the light aromatics column off gas it is burnt off in the flare system. Stream 8b is the sum of stream 8c which is the reflux and stream 8d which is the distillate from the aromatics column. Its pressure is 60 psig and it is recycled into the top of the light aromatics column as it contains p-xylenes to maintain efficient distillation [3, 13].

## 3. RESULT AND DISCUSSION

### 3.1. A material balance on Recovery phase

Consider the general material balance equation

$$\text{input} - \text{output} + \text{generation} = \text{accumulation} + \text{consumption} \quad (1)$$

The process is assumed to run on steady-state and therefore there is no accumulation in any of the designed equipment. Also, there is no reaction carried out unless otherwise stated therefore generation and consumption are both assumed to be zero elsewhere [13, 14].

### Material balance on first stage crystallization process

Overall balance beyond chiller

$$m_1 + m_{17} = m_2$$

Component balance beyond chiller

$$m_{1A} + m_{17A} = m_{2A}$$

$$m_{1B} + m_{17B} = m_{2B}$$

$$m_{1C} + m_{17C} = m_{2C}$$

$$m_{1D} + m_{17D} = m_{2D}$$

Overall balance on junction connecting 2 and 3

$$m_2/2 = m_3$$

Component balance on junction connecting 2 and 3

$$m_{2A}/2 = m_{3A}$$

$$m_{2B}/2 = m_{3B}$$

$$m_{2C}/2 = m_{3C}$$

$$m_{2D}/2 = m_{3D}$$

Table 3. Material balance results beyond chiller.

Stream ID Description	1	2	3
	Mixed Xylenes	Feed to 1 <sup>st</sup> stage crystallizer	Feed to 1 <sup>st</sup> crystallizer
Ethyl Benzene	2405.7	2687	1343
Para - xylene	8283	9251	4625
Meta - xylene	187341.4	20925	10462
Ortho - xylene	3577.2	3995	1997
Total	33000	36859.63	18429.815

Overall mass balance on crystallizers in series

$$m_3 = m_4$$

Component balance on crystallizers in series

$$m_{3A} = m_{4A}; m_{3B} = m_{4B}; m_{3C} = m_{4C}; m_{3D} = m_{4D}$$

Overall mass balance on centrifuge

$$m_4 + m_{6a}/2 - m_6/2 = m_5$$

Component balance on centrifuge

$$m_{4A} + m_{6aA}/2 - m_{6A}/2 = m_{5A}$$

$$m_{4B} + m_{6aB}/2 - m_{6B}/2 = m_{5B}$$

$$m_{4C} + m_{6aC}/2 - m_{6C}/2 = m_{5C}$$

$$m_{4D} + m_{6aD}/2 - m_{6D}/2 = m_{5D}$$

**Table 4. Material balance on crystallizers in series**

Stream ID Description	4	5	6	6a
	Feed to 1 <sup>st</sup> stage centrifuge	Feed to 1 <sup>st</sup> stage melt tank	Feed to 1 <sup>st</sup> stage filtrate surge drum	Recycle to 1 <sup>st</sup> stage centrifuge
Ethyl Benzene	1343.60	313.58	2865.495	573.098
Paraxylene	4625.69	990.64	4180.251	836.05
Meta - xylene	10462.61	2443.113	22384.57	4476.9143
Ortho-xylene	1997.792	466.6144	4281.39	856.28
Total	18429.81	4213.96	33711.70	6742.34

Overall mass balance on first stage melt tank

$$2m_5 + m_{7a} = m_7$$

Component balance on first stage melt tank

$$2m_{5A} + m_{7aA} = m_{7A}$$

$$2m_{5B} + m_{7aB} = m_{7B}$$

$$2m_{5C} + m_{7aC} = m_{7C}$$

$$2m_{5D} + m_{7aD} = m_{7D}$$

Overall mass balance on crystallizers in parallel

$$(m_{7b} + m_{16})/2 = m_{7c}$$

Component balance on crystallizers in parallel

$$(m_{7bA} + m_{16A})/2 = m_{7cA}$$

$$(m_{7bB} + m_{16B})/2 = m_{7cB}$$

$$(m_{7bC} + m_{16C})/2 = m_{7cC}$$

$$(m_{7bD} + m_{16D})/2 = m_{7cD}$$

**Material balance on second stage crystallizer**

Overall mass balance on second stage centrifuge

$$m_{8a} + m_{15a} - m_9 = m_{10}$$

Component balance on second stage centrifuge

$$m_{8aA} + m_{15aA} - m_{9A} = m_{10A}$$

$$m_{8aB} + m_{15aB} - m_{9B} = m_{10B}$$

$$m_{8aC} + m_{15aC} - m_{9C} = m_{10C}$$

$$m_{8aD} + m_{15aD} - m_{9D} = m_{10D}$$

Mass balance on second stage melt tank

$$m_{10} + m_{12} = m_{11}$$

Component balance on second stage centrifuge

$$m_{10A} + m_{12A} = m_{11A}$$

$$m_{10B} + m_{12B} = m_{11B}$$

$$m_{10C} + m_{12C} = m_{11C}$$

$$m_{10D} + m_{12D} = m_{11D}$$

Overall mass balance on junction post melt tank second stage

$$m_{11} = m_{12} + m_{13}$$

Component balance on junction post melt tank second stage

$$m_{11A} = m_{12A} + m_{13A}$$

$$m_{11B} = m_{12B} + m_{13B}$$

$$m_{11C} = m_{12C} + m_{13C}$$

$$m_{11D} = m_{12D} + m_{13D}$$

Overall mass balance on recycle surge tank

$$m_9 = m_{14} = m_{15a} + m_{15b}$$

Component balance on recycle surge tank

$$m_{9A} = m_{14A} = m_{15aA} + m_{15bA}$$

$$m_{9B} = m_{14B} = m_{15aB} + m_{15bB}$$

$$m_{9C} = m_{14C} = m_{15aC} + m_{15bC}$$

$$m_{9D} = m_{14D} = m_{15aD} + m_{15bD}$$

**Table 5. Material balance results of crystallizers in parallel**

Stream ID Description	5	7	7a	7b	7c
	Feed to melt tank	Discharge melt tank	Recycle to melt tank	To 2 <sup>nd</sup> stage crystallizer	Feed to 2 <sup>nd</sup> stage crystallizer
Ethyl benzene	313.5867	196.53	157.22	39.31	100.70
Paraxylene	990.6487	11932.24	9545.79	2386.45	6114.25
Meta - xylene	2443.113	1586.29	1269.03	317.26	812.84
Ortho - xylene	466.614	308.83	247.07	61.78	158.25
Total	4213.96	14037.93	11230.34	2807.59	7193.24

**Table 6. Material balance result of second stage centrifuge.**

Stream ID Description	8a	9	10	11	12
	To 2 <sup>nd</sup> stage centrifuge	To recycle surge drum	Discharge from centrifuge	Discharge from melt tank	Recycle to melt tank
Ethyl benzene	201.41	369.92	40.69	3.058	2.45
Paraxylene	12228.504	7710.43	2454.15	3027.69	2422.15
Meta - xylene	1625.67	2913.08	328.33	24.47	19.57
Ortho - xylene	316.50	566.43	63.92	3.06	2.45
Total	14386.47	11559.87	2889.97	3058.27	2446.61

**Table 7. Material balance results of recycle surge tank**

Stream ID Description	13	14	15a	15b	16	17
	To test tank	Discharge from the surge tank	Cold rinse to 2 <sup>nd</sup> stage	Recycle	Recycle to 2 <sup>nd</sup> stage Crystallizer	Recycle to 1 <sup>st</sup> stage crystallizer
Ethylbenzene	0.612	536.99	42.96	494.03	370.52	123.51
Paraxylene	605.54	11192.93	895.43	10297.49	7723.12	2574.37
Meta - xylene	4228.812	338.30	3890.51	328.33	2917.88	972.63
Ortho - xylene	0.612	822.27	65.78	756.49	567.36	189.12
Total	611.65	16781	1342.48	15438.52	11578.89	3859.63

**A material balance on Isomerization phase**

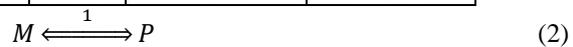
**A material balance on Reactor**

General material balance equation:

$$input + generation = output$$

When considering steady-state condition the term of accumulation tends to zero. Hence; *Input+generation =output*

The major reaction scheme is given below:



A thorough study of the kinetics of the reactions have been performed, results from polymath are published in chapter 6 designing and calculations. The results refer only to the exiting flow rates of meta-xylene, para-xylene, ortho-

xylene, tri-methylbenzene, toluene and all other species are considered as inert. Reacting component meta-xylene for 29.19% conversion [14, 15].

$$F_{m@discharge} = 298 - (298 \times 29.19/100) = 211 \text{ moles/hr}$$

Reacting component para xylene: for 65% selectivity of p-xylene

$$F_{px@discharge} = 86 + (298 - 211) \times 65/100 = 142.58 \text{ moles/hr}$$

Reacting component ortho xylene: for 33.4% selectivity of o-xylene

$$F_{ox@discharge} = 23 + (298 - 211) \times 33.4/100 = 52.07 \text{ moles/hr}$$

Meta xylene is converted into toluene and tri-methyl benzene in equal amounts; Reacting component Tri-methyl benzene:

$$F_{tmb@discharge} = \{ [100 - (65 + 33.4)] / 100 \} \times (298 - 211/2) = 0.4772 \text{ moles/hr}$$

Reacting component Toluene:

$$F_{tol@discharge} = 2.3 + 0.4772 = 2.7772 \text{ moles/hr}$$

The presence of hydrocarbons in the reactor is probable of resulting in coking of the catalyst within the reactor, the reactor design time has allowed for a calculation of coke formation and simultaneous de-coking of the catalyst with the help of Hydrogen [16, 17].

$$\% \text{ coke} = e^{-\alpha t} \quad (5)$$

$$\text{where; } \alpha = 0.959 \text{ s}^{-1}, t = 5.513 \text{ s}$$

$$\% \text{ coke} = e^{-(0.959 \times 5.513)} = 5.052 \times 10^{-3}$$

$$\text{Moles of coke} = 5.052 \times 10^{-3} \times 4420.8 = 22.335 \text{ moles/hr}$$

Assumed thermal cracking of the hydrocarbons components as shown in Table 8.

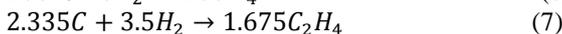
**Table 8: Thermal cracking of hydrocarbons.**

Specie	C <sub>4</sub>	C <sub>5</sub>	C <sub>6</sub>	C <sub>9</sub>
Cracked moles/hr	0.646	0.05	3.1	0.1

$$\text{Total moles of Carbon} = 4 \times (0.646) + 5 \times (0.05) + 6 \times (3.1) + 9 \times (0.1) = 22.335 \text{ moles/hr}$$

$$\text{Total moles of H}_2 = 0.5 \times 10 \times 0.646 + 12 \times 0.05 + 14 \times 3.1 + 20 \times 0.1 = 26.23 \text{ moles/hr}$$

Design feed of the reactor is such that the catalyst is recovered simultaneously, that is de-coking, by hydrogen within the reactor. Expected reactions involved in de-coking are as follows:



$$\text{Total moles of H}_2 \text{ consumed in de-coking: } (40 + 3.5025) = 43.5025 \text{ moles/hr}$$

Additional moles of Hydrogen consumed:

$$43.5025 - 26.23 = 17.2725 \text{ moles/hr}$$

All relevant reactions within the reactor for material balance have already been mentioned above, the rest of the species in the feed are considered inert at the reactor condition.

**Table 9. Material balance result of reactor**

Component	Reactor charge (moles/hr)	Reactor discharge (moles/hr)
H <sub>2</sub>	3318.4	3301.1275
C <sub>1</sub>	623.4	643.4
C <sub>2</sub>	13.9	15.0675
C <sub>3</sub>	6.4	6.4
C <sub>4</sub>	1.4	0.754
C <sub>5</sub>	0.1	0.05
C <sub>6</sub>	3.1	0
B	0.6	0.6
To	2.3	2.7772
Ethyl benzene	43.8	43.8
Para xylene	86.3	142.587
Meta xylene	298	211
Ortho xylene	23	52.0717
C <sub>9</sub>	0.1	0
Tri-methyl benzene	0	0.4772
Total	4420.8	4419.55

### A material balance on flash drum

To solve material balance on flash drum refer to the simplified form of Rachford-Rice equation mentioned below and for the method of determining K-values at T = 95°F and P = 140psig for an assumed vapor to feed a fraction of 0.9 that is [14, 17]:

$$v' = V/F \quad (8)$$

where; V = Vapor flow rate from flash drum, F = Feed flow rate, v' = vapor to feed fraction. Rachford- Rice equation:

$$\sum_{i=1}^{N_{co}} \frac{(K_i - 1) * z_i}{1 + (K_i - 1) * v'} \quad (9)$$

where; z<sub>i</sub> = fraction of component i in feed, y<sub>i</sub> = fraction of component i in vapor. x<sub>i</sub> = fraction of component i in liquid.

$$\text{General Balance equation: } F = V + L \quad (10)$$

$$\text{Component Balance equation: } z_i \times F = y_i \times V + x_i \times L$$

$$z_i = y_i \times v' + x_i \times (1 - v')$$

$$\text{Using the following relation: } y_i = K_i \times x_i$$

$$z_i = (K_i \times x_i \times v') + x_i \times (1 - v')$$

$$\text{And } x_i = z_i / [1 + (K_i - 1) \times v']$$

Table 11 shows the z<sub>i</sub> values determined from the material balance beyond the reactor and the K-values as determined.

**Table 10. Calculated values of z<sub>i</sub> and K<sub>i</sub>**

Component	z <sub>i</sub>	K <sub>i</sub>
H <sub>2</sub>	0.749	175.257
C <sub>1</sub>	0.146	19.60
C <sub>2</sub>	0.00341	4.47
C <sub>3</sub>	0.00145	1.401
C <sub>4</sub>	0.00017	0.4212
C <sub>5</sub>	0.000011	0.1461
B	0.00013	0.0204
Toluene	0.00063	0.00646
Ethyl benzene	0.0099	0.0403
Para xylene	0.0323	0.002109
Meta xylene	0.0478	0.002008
Ortho xylene	0.0118	0.001618
Tri-methyl benzene	0.000108	0.0003

**Table 11. Gas and liquid composition beyond flash drum**

Component	$x_i$	$y_i$
H <sub>2</sub>	0.00473	0.8318
C <sub>1</sub>	0.00823	0.161
C <sub>2</sub>	0.000829	0.00370
C <sub>3</sub>	0.00106	0.00148
C <sub>4</sub>	0.0003571	0.000157
C <sub>5</sub>	0.0000490	0.000007
Benzene	0.00128	0.0000261
Toluene	0.00595	0.000038
Ethyl benzene	0.0728	0.00294
Para xylene	0.3175	0.00066
Meta xylene	0.4703	0.00094
Ortho xylene	0.11647	0.000188
Tri-methyl benzene	0.00108	0.00000032

Using the set of equations mentioned earlier and the Table 10 mole fractions for the liquid stream and the vapor stream leaving the flash drum has been determined when  $v' = 0.9$ ,  $T = 95^\circ\text{F}$  and  $P = 140\text{psig}$ . The result is displayed in the Table 11.

To determine the molar flow rates of the species consider  $v' = 0.9$ ,  $V/F = 0.9$ .

$$V = 0.9 \times 4406.55 = 3965.895 \text{ moles/hr}$$

$$L = F - V = 4406.55 - 3965.895 = 440.655 \text{ moles/hr}$$

The resulting molar flow rates of the species are in Table 12.

**Table 12. Molar flow rates of components**

Component	Liquid flow rate (moles/hr)	Vapor Flow rate (moles/hr)
H <sub>2</sub>	2.08	3298.8
C <sub>1</sub>	3.62	638.5
C <sub>2</sub>	0.365	14.67
C <sub>3</sub>	0.467	5.86
C <sub>4</sub>	0.157	0.622
C <sub>5</sub>	0.021	0.028
Benzene	0.564	0.103
Toluene	2.62	0.15
Ethyl benzene	32.07	11.6
Para xylene	139.9	2.61
Meta xylene	207.24	3.72
Ortho xylene	51.32	0.745
Tri-methyl benzene	0.475	0.0012

**Material Balance on Distillation Column**

$$\text{Feed} = \text{Distillate} + \text{Bottoms product}$$

$$F = D + B$$

$$440.7 = D + B$$

For Table 13 bottom and distillate stream compositions.

**Table 13. Molar composition desired of distillation column**

Components	Distillate	Bottom
H <sub>2</sub>	0	0
C <sub>1</sub>	0	0
Toluene	0.1	0
Ethyl Benzene	0.129	0.070
Para-Xylene	0.302	0.323
Meta-Xylene	0.43	0.4837
Ortho-Xylene	0.036	0.1228
Total	1	1

$$440.7 = D + B$$

$$440.7 X_F = X_D D + X_B B$$

Solving 1 and 2 for any specie;  $D = 23.12 \text{ Lbmol/hr}$ ,  $B = 410.53 \text{ Lbmol/hr}$ ,

$$\text{Off gases} = F - D - B = 440.7 - 23.12 - 410.53 = 6.96 \text{ Lbmol/hr}$$

For a reflux ratio of 15  $R = 15 * D$

**Table 14. Molar flow rates distillate and reflux stream**

Components	Distillate	Bottom
H <sub>2</sub>	0	0
C <sub>1</sub>	0	0
Toluene	2.323	34.845
Ethyl Benzene	3	45
Para-Xylene	6.998	104.97
Meta-Xylene	9.957	149.355
Ortho-Xylene	0.8513	12.7695
Total	23.129	346.93

Results from the overall material balance for the isomerization unit have been tabulated in Table 15 a and b.

**Energy Balance**

**General energy balance equation**

Rate of energy accumulation in the system.

$$\sum_{input \text{ stream}} m_j (\hat{U}_j + \frac{u_j^2}{2} + gz_j) - \sum_{output \text{ stream}} m_j (\hat{U}_i + \frac{u_i^2}{2} + gz_i) + Q - W = \frac{dE_{sys}}{dt} \tag{11}$$

The following performed energy balances the process is assumed to run on steady state and therefore there is no energy accumulation in any of the designed equipment.

**Table 15 a). Overall material balance isomerization unit**

Steam ID	1	2	3	4
Description	Xylene Feed	Total Gas	Total Reactor	Reactor
	From Tank	To Reactor	Charge	Effluent
Total Lbs/Hr	46896	18961	65857	65857
Molecular weight	106	4.76	14.8	14.9
H <sub>2</sub>	0	3318.4	3318.4	3301.1275
C <sub>1</sub>	0	623.4	623.4	643.4
C <sub>2</sub>	0	13.9	13.9	15.0675
C <sub>3</sub>	0	6.4	6.4	6.4
C <sub>4</sub>	0	1.4	1.4	0.754
C <sub>5</sub>	0	0.1	0.1	0.05
C <sub>6</sub>	0	3.1	3.1	0
Benzene	0	0.6	0.6	0.6
Toulene	1.4	0.9	2.3	2.7772
Ethyl-Benzene	42.7	1.1	43.8	43.8
Para-Xylene	84	2.3	86.3	142.587
Meta-Xylene	293	5	298	211
Ortho-Xylene	21.4	1.6	23	52.0717
C <sub>9</sub> + Aromatics	0	0.1	0.1	0
Total	442.5	3978.3	4420.8	4419.6349
Steam Id	5	6	7	8a
Description	Light Aromatic	Flash Drum Bleed	Light Aromatic	Light Aromatic
	Column Feed	Gas To Fuel	Bottom Product	Off Gas
Total Lbs/Hr	46156.4352	19700.5648	43580	150
Molecular weight	104.8	4.95	106.29	21.55
H <sub>2</sub>	2.08	3298.8	0	2.079

C <sub>1</sub>	3.62	638.5	0	3.584
C <sub>2</sub>	0.365	14.67	0	0
C <sub>3</sub>	0.467	5.86	0	0
C <sub>4</sub>	0.157	0.622	0	0
C <sub>5</sub>	0.021	0.028	0	0
C <sub>6</sub>	0	0	0	0
Benzene	0.564	0.103	0	0
Toulene	2.62	0.15	0	0.2856
Ethyl-Benzene	32.07	11.6	28.89	0.169
Para-Xylene	139.9	2.61	132.6	0.3506
Meta-Xylene	207.24	3.72	198.6	0.4945
Ortho-Xylene	51.32	0.745	50.44	0
C <sub>9</sub> + Aromatics	0	0	0	0
Total	440.424	3977.408	410.53	6.9627

Table 15 b). Overall material balance isomerization unit

Steam Id	8c	8d
	Light Aromatic Column Reflux	Light Aromatic Column Distillate
Description		
Total Lbs/Hr	36390	2426
Molecular weight	104.9	104.88
H <sub>2</sub>	0	0
C <sub>1</sub>	0	0
C <sub>2</sub>	0	0
C <sub>3</sub>	0	0
C <sub>4</sub>	0	0
C <sub>5</sub>	0	0
C <sub>6</sub>	0	0
Benzene	0	0
Toulene	34.845	2.323
Ethyl-Benzene	45	3
Para-Xylene	104.97	6.998
Meta-Xylene	149.355	9.957
Ortho-Xylene	12.7695	0.8513
C <sub>9</sub> + Aromatics	0	0
Total	346.9395	23.1293

Also, the system is assumed to be of the close type, therefore, there is no heat flow into the system from the surroundings and also the shaft work is neglected for the ease of calculations. The kinetic and potential energies of the components are also assumed to have no effect on overall heat transfer between the two streams of exchangers. Thus the above equation can be simplified as [14, 17]:

$$\sum_{input\ stream} m_j(\hat{U}_j) = \sum_{output\ stream} m_i(\hat{U}_i) \quad (12)$$

$$m_i \times cp_i \times \Delta T_i = m_o \times cp_o \times \Delta T_o$$

$$Q_i = Q_o$$

#### Energy Balance on exchanger (E - 200)

$$Q_1 = m_1 \times Cp_1 \times \Delta T \quad (13)$$

where: Stream 1 is the main process and Stream 2 is the hot reactor effluent.

M<sub>1</sub> = number of moles × Molecular Weight

where: MW = 14.8 (from HYSYS), Cp<sub>1</sub> = 0.73 Btu/lb.°F (from HYSYS), moles = 4420.8 moles/hr.

$$M_1 = 4420.8 \times 14.8 = 65857 \text{ lbhr}$$

$$\Delta T = T_2 - T_1$$

For reactor effluent stream which is being heated T<sub>1</sub> = 95°F, T<sub>2</sub> = 210°F

$$Q_2 = M_2 \times Cp_2 \times \Delta T \quad M_2 = 65857 \text{ lb/hr}$$

$$Cp_2 = 0.536 \text{ BTU/lb.}^\circ\text{F (from HYSYS)}$$

$$\Delta T = 210 - 95 = 115^\circ\text{F}$$

$$Q_2 = (Cp_2 \times M_2) \times \Delta T = 26.19 \text{ MMBtu/hr}$$

For the purpose of calculation approximation of outlet temperature of the cold stream: Since Q<sub>1</sub> = Q<sub>2</sub>, Q<sub>1</sub> = 65857 × 0.73 × (ΔT) and ΔT = 544.8°F

$$\Delta T = T_2 - T_1$$

$$T_2 = 700^\circ\text{F}$$

#### Energy Balance on exchanger (E - 201)

$$Q_1 = m_1 \times Cp_1 \times \Delta T$$

where: Stream 1 is the main process stream.

M<sub>1</sub> = number of moles × Molecular Weight

where: MW = 14.9 (from HYSYS), Cp<sub>1</sub> = 0.9138 Btu/lb.°F (from HYSYS), moles = 4419.55 moles/hr,

$$m_1 = 4419.55 \times 14.9 = 65857.25 \text{ lb/hr}$$

$$\Delta T = T_2 - T_1$$

For process stream which is being cooled T<sub>1</sub> = 210°F, T<sub>2</sub> = 135°F

$$\Delta T = 135 - 210 = -75^\circ\text{F (since heat is being removed from the stream)}$$

$$Q_1 = 65857.25 \times 0.9138 \times (-75) = 4.51 \text{ MMBTU/hr}$$

#### Energy Balance on exchanger (E - 202)

$$Q_1 = M_1 \times Cp_1 \times \Delta T$$

where: Stream 1 is the main process and stream 2 is the water stream.

M<sub>1</sub> = Number of moles \* Molecular Weight

where: MW = 14.9 (from HYSYS) Cp<sub>1</sub> = 0.9138 Btu/lb.°F (from HYSYS) moles = 4419.55 moles/hr

$$M_1 = 4419.55 \times 14.9 = 65857.25 \text{ lbhr}$$

$$\Delta T = T_2 - T_1$$

For process stream which is being cooled: T<sub>1</sub> = 135°F, T<sub>2</sub> = 95°F

$$\Delta T = 95 - 135 = -40^\circ\text{F (since heat is being removed from the stream)}$$

$$Q_1 = 65857.25 \times 0.9138 \times (-40) = 2.406 \text{ MMBtu/hr}$$

For the purpose of calculation of water flow rate around the trim cooler:

$$\text{Since } Q_1 = Q_2$$

$$Q_2 = M_2 \times Cp_2 \times \Delta T$$

$$Cp_2 = 1.0303 \text{ BTU/lb.}^\circ\text{F (from HYSYS)}$$

$$\Delta T = 100 - 81 = 19^\circ\text{F}$$

$$M_2 = Q_2 / (Cp_2 \times \Delta T) = 123419.5 \text{ lb/hr} = 246 \text{ GPM}$$

#### Energy Balance on exchanger (E - 203)

$$Q_1 = M_1 \times Cp_1 \times \Delta T$$

where: Stream 1 is the main process and stream 2 is the bottom discharge of the distillation column.

$M_1 =$  Number of moles  $\times$  Molecular Weight

where: MW = 104.8 (from HYSYS),  $C_{p1} = 0.3914$  Btu/lb. $^{\circ}$ F (from HYSYS), moles = 440.424 moles/hr

$M_1 = 440.424 \times 104.8 = 46156.25$  lb/hr

$\Delta T = T_2 - T_1$

For process stream which is being heated:  $T_1 = 95^{\circ}$ F,  $T_2 = 268^{\circ}$ F

$\Delta T = 268 - 95 = 173^{\circ}$ F

$Q_1 = 46156.25 \times 0.3914 \times (173) = 3.12$  MMBtu/hr

For the purpose of calculation approximation of outlet temperature of the hot stream: Since  $Q_1 = Q_2$

$Q_2 = M_2 \times C_{p2} \times \Delta T$

$M_2 = 43580$  lb/hr

$C_{p2} = 0.4$  BTU/lb. $^{\circ}$ F (from HYSYS)

$\Delta T = Q_2 / (C_{p2} \times m_2)$

$T_2 = 143^{\circ}$ F

#### Energy Balance on exchanger (E - 206)

$Q_1 = M_1 \times C_{p1} \times \Delta T$

Where: Stream 1 is the main process stream  $C_{p1} = 0.46$  Btu/lb. $^{\circ}$ F (from HYSYS),  $m_1 = 38966$  lb/hr

$\Delta T = T_2 - T_1$

For process stream which is being cooled:  $T_1 = 196^{\circ}$ F,  $T_2 = 145^{\circ}$ F

$\Delta T = 145 - 196 = -51^{\circ}$ F (since heat is being removed from the stream)

$Q_1 = 38966 \times 0.46 \times (-51) = 0.91$  MMBtu/hr

#### Energy Balance on exchanger (E - 207)

$Q_1 = M_1 \times C_{p1} \times \Delta T$

where: Stream 1 is the main process and stream 2 is the water stream

$M_1 =$  Number of moles  $\times$  Molecular Weight

$C_{p1} = 0.46$  Btu/lb. $^{\circ}$ F (from HYSYS),  $m_1 = 38966$  lb/hr

$\Delta T = T_2 - T_1$

For process stream which is being cooled  $T_1 = 145^{\circ}$ F,  $T_2 = 100^{\circ}$ F

$\Delta T = 100 - 145 = -45^{\circ}$ F (since heat is being removed from the stream)

$Q_1 = 38966 \times 0.46 \times (-45) = 0.80$  MMBtu/hr

For the purpose of calculation of water flow rate around the trim cooler:

Since  $Q_1 = Q_2$

$Q_2 = M_2 \times C_{p2} \times \Delta T$

$C_{p2} = 1.0303$  BTU/lb. $^{\circ}$ F (from HYSYS)

$\Delta T = 100 - 81 = 19^{\circ}$ F

$M_2 = Q_2 / (C_{p2} \times \Delta T) = 41203$  lb/hr = 82 GPM

#### Energy Balance on first stage crystallizer (C-100)

$Q_1 = M_1 \times C_{p1} \times \Delta T$

where: Stream 1 is the main process and Stream 2 is the hot reactor effluent.

$M_1 =$  Number of moles  $\times$  Molecular Weight

$C_{p1} = 0.405$  Btu/lb. $^{\circ}$ F (from HYSYS),  $m_1 = 18000$  lb/hr

$\Delta T = T_2 - T_1$

$T_1 = -11^{\circ}$ F,  $T_2 = -45^{\circ}$ F,  $\Delta T = -34^{\circ}$ F,  $Q_1 = -247860$  Btu/hr

For the purpose of determining the coolant (ethylene) outlet temperature:

$Q_2 = m_2 \times C_{p2} \times \Delta T$

$m_2 = 15000$  lb/hr,  $C_{p2} = 0.31$  BTU/lb. $^{\circ}$ F (from HYSYS),

$\Delta T = ?$ ,  $T_1 = -71^{\circ}$ F,  $T_2 = -17.69^{\circ}$ F

$\Delta T = Q_2 / (C_{p2} \times m_2)$

#### Energy Balance on first stage crystallizer (C-101)

$Q_1 = M_1 \times C_{p1} \times \Delta T$

Where: Stream 1 is the main process and Stream 2 is the hot reactor effluent.

$M_1 =$  Number of moles  $\times$  Molecular Weight

$C_{p1} = 0.326$  Btu/lb. $^{\circ}$ F (from HYSYS),  $m_1 = 18000$  lb/hr,  $T_1 = -45^{\circ}$ F,  $T_2 = -73^{\circ}$ F

$\Delta T = T_2 - T_1 = -28^{\circ}$ F

$Q_1 = -164304$  Btu/hr

For the purpose of determining the coolant (ethylene) outlet temperature:  $Q_2 = m_2 \times C_{p2} \times \Delta T$

$m_2 = 15000$  lb/hr,  $C_{p2} = 0.286$  BTU/lb. $^{\circ}$ F (from HYSYS),

$\Delta T = ?$ ,  $T_1 = -105^{\circ}$ F

$\Delta T = Q_2 / (C_{p2} \times m_2)$

$T_2 = -66.7^{\circ}$ F

#### Energy Balance on first stage crystallizer (C-102)

$Q_1 = M_1 \times C_{p1} \times \Delta T$

Where: Stream 1 is the main process and Stream 2 is the hot reactor effluent.

$M_1 =$  Number of moles  $\times$  Molecular Weight

$C_{p1} = 0.718$  Btu/lb. $^{\circ}$ F (from HYSYS),  $m_1 = 10375$  lb/hr,  $T_1 = 64^{\circ}$ F,  $T_2 = 25^{\circ}$ F

$\Delta T = T_2 - T_1 = -39^{\circ}$ F

$Q_1 = -290520$  Btu/hr

For the purpose of determining the coolant (propane) outlet temperature:  $Q_2 = m_2 \times C_{p2} \times \Delta T$

$m_2 = 9000$  lb/hr,  $C_{p2} = 0.556$  BTU/lb. $^{\circ}$ F (from HYSYS),

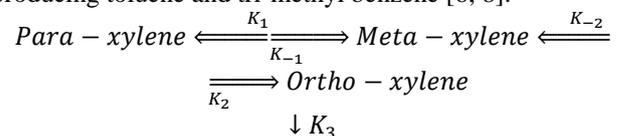
$\Delta T = ?$ ,  $T_1 = -1^{\circ}$ F

$\Delta T = Q_2 / (C_{p2} \times m_2)$

$T_2 = -59^{\circ}$ F

#### REACTION KINETICS OF PARA XYLENE

It is known through research that meta-xylene undergoes two main reactions over zeolite catalysts. Isomerization is the reaction which produces para-xylene and ortho-xylene while disproportionation reaction is recognized as the one producing toluene and tri-methyl benzene [6, 8].



Para-xylene increased selectivity is reportedly favored by the use of ZSM-5 zeolite catalyst which enhances the probability of isomerization reaction at the expense of disproportionation reaction also being more selective towards para-xylene than ortho-xylene. Furthermore, the modification of zeolite or its pretreatment was found to further boost the catalyst shape selectivity [10, 18].

Pre-coking, for instance, is professed to build para-xylene selectivity up to 70-80%. As to coking, the wonder is to such an extent that the coke specifically stores on the zeolite outside surface covering the outer dynamic locales by presenting the appropriate particles. These specific huge molecules than can't infiltrate into the catalyst structure consequently they will undoubtedly respond on the outside empty locales favoring coke arrangement which covers those destinations utilized for para-xylene change which is an undesired optional response. Since coke stores just on the outer structure, it is expected that the inward destinations remain undisturbed. In pre-coking, the catalyst is at first reached with certain feedstock at a specific response condition to store a specific measure of coke on the catalyst. It must be remembered that an enormous measure of the coke can deactivate even the inside active destinations. Along these lines to keep away from a negative impact of the pre-coking process, it must be

deliberately controlled [7].

**Conversion of meta-xylene** It is conspicuous that meta-xylene conversion increments with both response temperature and time. Research recommends for all response temperatures, the conversion will fundamentally rise with time as appeared in Figure 4.

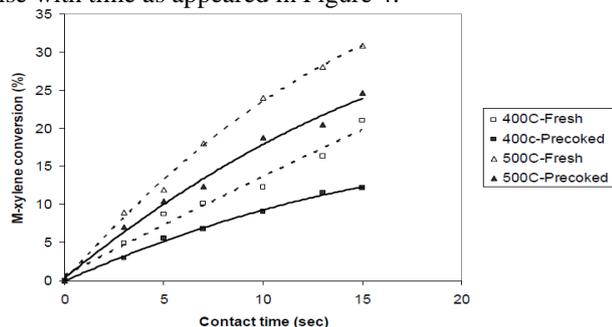


Fig. 4. Meta-xylene conversion concerning contact time and temperature

#### The ratio of Isomerization to Disproportionate (I/D)

The change of m-xylene over zeolite catalyst continues as two main responses; isomerization and disproportionation. Disproportionation reaction requires two molecules of m-xylene reactant and is a massive response. Therefore, disproportionation is conspicuous just on huge pore size zeolite that can house these intermediates. It must be referenced that few scientists recommended that D/I proportion on ZSM-5 approaches zero because of its little pores. It very well may be seen from Figure 5 that I/D decline with temperature while change moderately affects this proportion. The decline of I/D with temperature demonstrates that disproportionation response is more sensitive to temperature than isomerization. This perception compliments the way that disproportionation requires higher activation energy when contrasted with isomerization response [9].

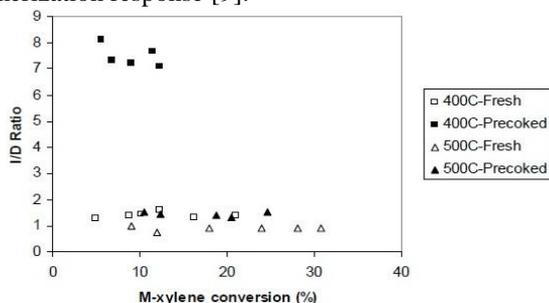
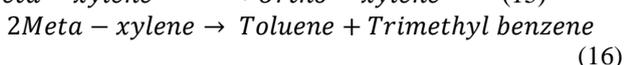
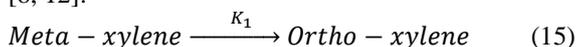


Fig. 5. The effect of meta-xylene conversion, catalyst pre-coking and reaction temperature on I/D ratio.

Figure 5 also shows the impact of catalyst deactivation on I/D proportion. I/D proportion for the halfway deactivated catalyst changes radically with temperature. The reduction in disproportionation can be effectively clarified on the premise that this response requires two contiguous dynamic destinations to happen. The increase in I/D proportion with partial coking deactivation bringing about a portion of the dynamic destinations being secured by coke, diminishing disproportionation selectivity which is a bigger number of locales requesting than isomerization response [8, 9].

#### Kinetic Model Development

To develop an appropriate kinetic model presenting the general conversion of m-xylene, the reaction are given as [8, 12]:



where;  $K_1$ =Reaction rate constant for the forward m-p reaction ( $\text{ft}^3/\text{lb cat.h}$ ),  $K_{-1}$ = Reaction rate constant for the backward p-m reaction ( $\text{ft}^3/\text{lb cat.h}$ ),  $K_2$  =Reaction rate constant for the forward m-o reaction ( $\text{ft}^3/\text{lb cat.h}$ ),  $K_{-2}$ = Reaction rate constant for the backward o-m reaction ( $\text{ft}^3/\text{lb cat.h}$ ) and  $K_3$ =Reaction rate constant for the disproportionation reaction ( $\text{ft}^3/\text{lb cat.h}$ ).

$$(K_{eq})_{mp} = k_1/(k_{-1})$$

$$(K_{eq})_{mo} = k_2/(k_{-2})$$

Temperature-dependent equilibrium constants for the two responses. Though, an average value can be processed for the two constants, because the thermodynamic equilibrium concentrations of the xylenes remain consistent inside the temperature scope of this work. It was found from transformations of m-xylene over fresh and precoked ZSM-5, the fresh catalyst greater m-xylene conversion increased the selectivity of isomerization reaction and selectivity of p-xylene.

#### EQUIPMENT DESIGNING

##### Designing heat exchangers

The objective of heat exchanger design is to relate the inlet and outlet temperatures, the general heat transfer coefficient, the rate of heat transfer between the two liquids and its geometry.

$$\text{Heat balance: } Q = WC(T_1 - T_2) = wc(t_2 - t_1) \quad (17)$$

$$\text{True temperature difference } \Delta t: R = (T_1 - T_2)/(t_2 - t_1)$$

$$S = (t_2 - t_1)/(T_1 - t_1)$$

$$\Delta t = \text{LMTD} \times F_T$$

$$\text{Log Mean Temperature Difference (LMTD): } \text{LMTD} = (\Delta t_1 - \Delta t_2) / \ln(\Delta t_1 / \Delta t_2) \quad (18)$$

$$\text{Heat transfer surface: } A = a'' \times L \times N_t \quad (19)$$

$$\text{Overall design coefficient: } U_D = Q / (A \times \Delta t) \quad (20)$$

The heat exchanger E – 100 hot fluid mass flow rate 5580 lb/h, specific heat capacity 0.318 BTU/lb.°F, overall heat transfer co-efficient 60 (assuming), inlet temperature 105 °F, outlet temperature -10 °F and Q 1640000 BTU/h. The shell side pass is 3 and internal diameter 21.25 inch. The cold fluid mass flow rate 31727 lb/h, specific heat capacity 1.695, overall heat transfer co-efficient 60 (assuming), inlet temperature -59 °F and outlet temperature 72 °F. The tube side 16 BWG 1 inch, length 16 Ft, internal diameter 0.62 inch, outer diameter 0.75 inch and passes 6 [10].

Hot Fluid °F	Temperature °F	Cold Fluid °F	Difference °F
105	Higher	72	33
-10	Lower	-59	49
115	Differences	131	-16

Table 16 shows the operating and designing parameter heat exchanger E – 100. The heat exchanger E – 101 hot fluid mass flow rate 672.22 lb/h, specific heat capacity 0.318 BTU/lb.°F, overall heat transfer co-efficient 60 (assuming), inlet temperature 358 °F, outlet temperature 358 °F and Q 2500000 BTU/h. The shell side pass is 1 and the internal diameter 13.25 inch. The cold fluid mass flow rate 26800 lb/h, specific heat capacity 0.754, overall heat transfer co-efficient 60 (assuming), inlet temperature 100 °F and outlet temperature 170 °F. The tube side 52 BWG 16 inch, length 12 ft, internal diameter 0.582 inches, outer diameter 1 inch and passes 4.

Table 16. Operating and designing parameter heat exchanger E – 100.

Parameters	Calculated
LMTD ( $T_M$ )	40.47428407 °F
R & S Factors	
R	0.877862595
S	0.798780488

$F_T$	0.855
$\Delta t$	34.60551288 °F
Area (A)	789.8548832 ft <sup>2</sup>
Number of tubes ( $N_T$ )	251.4820693
<b>Calculation of <math>U_D</math></b>	
Shell ID	21.25 inch
Pitch	1" square pitch
Number of tubes	240
$U_D$	62.87051732 (Corrected)
<b>Shell Side</b>	
Baffle spacing (B)	4.25 inches
Flow Area ( $A_F$ )	0.156792535 ft <sup>2</sup>
Mass velocity (G)	35588.42907 lb/hr.ft <sup>2</sup>
Equivalent diameter ( $D_e$ )	0.079166667 Ft
Viscosity ( $\mu$ )	4.72142 lb/ft.h
Reynold Number (Re)	596.7309202
$J_H$ Factor	13
K	0.225
( $cp \times \mu / k$ )	1.882662241 BTU/hr.ft <sup>2</sup> .(°F/ft)
$h_o$	69.55941543 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
f	0.0038
SG	0.86
Number of crosses	45.17647059
$D_s$	1.770833333 ft
Pressure drop	0.108337774 psi
<b>Tube Side</b>	
Flow area per tube $A_F$	0.302 inch <sup>2</sup> /tube
$A_T$	0.083888889 inch <sup>2</sup>
Mass Velocity $G_T$	378202.649 lb/hr.ft <sup>2</sup>
Viscosity $\mu$	1.228634 lb/ft.h
Reynolds Number Re	15904.22388
$J_H$ Factor	50
K	0.149
( $cp \times \mu / k$ )	2.40880 BTU/hr.ft <sup>2</sup> .(°F/ft)
$h_i$	347.334453 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
Reynolds Number	15904.22388
F	0.00025
SG	0.85
Pressure drop	1.497478178 psi

Hot Fluid °F	Temperature °F	Cold Fluid °F	Difference °F
358	Higher	170	188
358	Lower	100	258
0	Differences	70	-70

Table 17 shows the operating and designing parameter heat exchanger E – 101.

Table 17. Operating and designing parameter heat exchanger E – 101.

Parameters	Calculated
LMTD $T_M$	221.1567228 °F
Average temperature $T_a$	185 °F
Area (A)	163.3632 ft <sup>2</sup>
<b>Calculation of <math>U_D</math></b>	
Shell inner dia	13.25 inch
Pitch	1.25" square pitch
Number of tubes	52
$U_D$	218.6189 BTU/hr.ft <sup>2</sup> .°F
<b>Shell Side</b>	
Baffle Spacing (B)	15 inches
Flow Area $A_F$	0.276041667 ft <sup>2</sup>
Mass Velocity G	2435.212075 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.0825 Ft
Viscosity $\mu$	0.0242 lb/ft.h
Reynolds Number Re	8301.859348
Rate of condensation of steam $R_s$	864.3 Btu/hr
<b>Pressure Drop</b>	
Reynold Number	8301.859348
F	0.002
SG	0.00123
No of Crosses	9.6
$D_s$	1.104166667 ft
Pressure Drop	0.023734488 Psi
<b>Tube Side</b>	

Flow area per tube $A_F$	0.4 inch <sup>2</sup> /tube
$A_T$	0.036111111 inch <sup>2</sup>
Mass Velocity $G_T$	742153.8462 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.0485 Ft
Viscosity $\mu$	1.3068 lb/ft.h
Reynolds Number Re	27543.97118
$J_H$ Factor	82
K	0.149
( $cp \times \mu / k$ )	1.877BTU/hr.ft <sup>2</sup> .(°F/ft)
$H_i$	472.8497 BTU/hr.ft <sup>2</sup> .°F
$U_c$	305.6381 BTU/hr.ft <sup>2</sup> .°F
$R_D$	0.001302 hr.ft <sup>2</sup> .F/Btu
<b>Pressure Drop</b>	
Reynolds Number	27543.97118
f	0.00022
SG	0.78
Pressure Drop	2.945404587 psi

The heat exchanger E – 102 hot fluid mass flow rate 344 lb/h, specific heat capacity 0.318 BTU/lb.°F, overall heat transfer coefficient 60 (assuming), inlet temperature 450 °F, outlet temperature 450 °F and Q 715000 BTU/h. The shell side pass is 1 and the internal diameter 13.25 inch. The cold fluid mass flow rate 26969 lb/h, specific heat capacity 0.67, overall heat transfer co-efficient 60 (assuming), inlet temperature -79 °F and outlet temperature -59 °F. The tube side 52 BWG 1.25 inch, length 16 ft, internal diameter 0.582 inches, outer diameter 1 inch and passes 4.

Hot Fluid °F	Temperature °F	Cold Fluid °F	Difference °F
450	Higher	-59	509
450	Lower	-79	529
0	Differences	20	-20

Table 18 shows the operating and designing parameter heat exchanger E – 102.

Table 18. Operating and designing parameter heat exchanger E – 102

Parameters	Calculated
LMTD $T_m$	518.9357 °F
Average Temperature $T_a$	-69 °F
Area A	217.817 ft <sup>2</sup>
<b>Calculation of <math>U_D</math></b>	
Shell ID	13.25 inch
Pitch	1.25" square pitch
Number of Tubes	52
$U_D$	164.12 BTU/hr.ft <sup>2</sup> .°F
<b>Shell Side</b>	
Baffle Spacing B	15 inches
Flow Area $A_F$	0.276041667 ft <sup>2</sup>
Mass Velocity G	1246.188 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.0825 ft
Viscosity $\mu$	0.0314 lb/ft.h
Reynolds Number Re	3267.977
Rate of condensation of steam $R_s$	1245 Btu/hr
<b>Pressure Drop</b>	
F	0.0023
SG	0.00123
Number of Crosses	12.8
$D_s$	1.104166667 ft
Pressure Drop	0.00953 psi
<b>Tube Side</b>	
Flow area per tube $A_F$	0.4 inch <sup>2</sup> /tube
$A_T$	0.0361111 inch <sup>2</sup>
Mass Velocity $G_T$	746833 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.0485 Ft
Viscosity $\mu$	1.3068 lb/ft.h
Reynolds Number Re	27717
$J_H$ Factor	90
K	0.234
( $cp \times \mu / k$ )	1.557BTU/hr.ft <sup>2</sup> .(°F/ft)
$H_i$	676 BTU/hr.ft <sup>2</sup> .°F
$U_c$	438.17 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
f	0.00022
SG	0.86
Pressure Drop	3.607 psi

The heat exchanger E – 203 hot fluid mass flow rate 43580 lb/h, specific heat capacity 0.4 BTU/lb.°F, overall heat transfer co-

efficient 65 (assuming), inlet temperature 322 °F, outlet temperature 145 °F and Q 3800000 BTU/h. The shell side pass is 4 and the internal diameter 27 inches. The cold fluid mass flow rate 46156 lb/h, specific heat capacity 0.3914, overall heat transfer co-efficient 65 (assuming), inlet temperature 95 °F and outlet temperature 268 °F. The tube side 52 BWG 1 inch, length 16 ft, internal diameter 0.62 inches, outer diameter 0.75 inch and passes 8. Table 19 shows the operating and designing parameter heat exchanger E – 203.

Hot Fluid °F	Temperature °F	Cold Fluid °F	Difference °F
322	Higher	268	54
145	Lower	95	50
177	Differences	173	4

Table 19. Operating and designing parameter heat exchanger E – 203

Parameters	Calculated
LMTD $T_M$	51.97434885 °F
R	1.023121387
S	0.762114537
$F_T$	0.9
$\Delta t$	46.77691397 °F
Area (A)	1249.794685 ft <sup>2</sup>
Number of tubes $N_T$	397.9224036
<b>Calculation of <math>U_D</math></b>	
Shell ID	27 inch
Pitch	1.0" square pitch
Number of Tubes	408
$U_D$	63.394557 BTU/hr.ft <sup>2</sup> .°F
<b>Shell Side</b>	
Baffle Spacing B	5.4 inches
Flow Area $A_F$	0.253125 ft <sup>2</sup>
Mass Velocity G	172167.9012 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.079166667 ft
Viscosity $\mu$	0.363 lb/ft.h
Reynolds Number Re	37548.096
$J_H$ Factor	110
K	0.0069
( $cp \times u/k$ )	2.7609 BTU/hr.ft <sup>2</sup> .(°F/ft)
$H_i$	26.469148 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
F	0.0017
SG	0.727
Number of Crosses	35.55555556
$D_s$	2.25 ft
Pressure Drop	1.341825392 psi
<b>Tube Side</b>	
Flow area per tube $A_F$	0.302 inch <sup>2</sup> /tube
$A_T$	0.106958333 inch <sup>2</sup>
Mass Velocity $G_T$	431532.5282 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.051666667 Ft
Viscosity $\mu$	1.2342 lb/ft.h
Reynolds Number Re	18065.01968
$J_H$ Factor	62
K	0.008
( $cp \times u/k$ )	3.923 BTU/hr.ft <sup>2</sup> .(°F/ft)
$H_i$	37.66256 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
f	0.00022
SG	0.86
Pressure Drop	2.260894661 psi

The heat exchanger E – 200 hot fluid mass flow rate 65857 lb/h, specific heat capacity 0.536 BTU/lb.°F, overall heat transfer co-efficient 73 (assuming), inlet temperature 950 °F, outlet temperature 210 °F and Q 45000000 BTU/h. The shell side pass is 4 and the internal diameter 35 inches. The cold fluid mass flow rate 65857 lb/h, specific heat capacity 0.73, overall heat transfer co-efficient 73 (assuming), inlet temperature 155 °F and outlet temperature 700 °F. The tube side 52 BWG 1 inch, length 20 ft, internal diameter 0.87 inches, outer diameter 0.75 inches and passes 8.

Hot Fluid °F	Temperature °F	Cold Fluid °F	Difference °F
950	Higher	700	250
210	Lower	155	55
740	Differences	545	195

Table 20 shows the operating and designing parameter heat exchanger E – 200.

Table 20. Operating and designing parameter heat exchanger E – 200

Parameters	Calculated
LMTD $T_M$	128.7870209 °F
R	1.357798165
S	0.685534591
$F_T$	0.84
$\Delta t$	108.1810976 °F
Area (A)	5698.207634 ft <sup>2</sup>
Number of tubes $N_T$	725.8863229
<b>Calculation of <math>U_D</math></b>	
Shell ID	35 inch
Pitch	1.0" square pitch
Number of Tubes	748
$U_D$	106.2086 BTU/hr.ft <sup>2</sup> .°F
<b>Shell Side</b>	
Baffle Spacing B	7 inches
Flow Area $A_F$	0.340277778 ft <sup>2</sup>
Mass Velocity G	193538.9388 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.079166667 ft
Viscosity $\mu$	1.21 lb/ft.h
Reynolds Number Re	12662.67161
$J_H$ Factor	62
K	0.138
( $cp \times u/k$ )	1.6750 BTU/hr.ft <sup>2</sup> .(°F/ft)
$h_o$	181.0306 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
F	0.002
SG	0.852
Number of Crosses	34.28571429
$D_s$	2.916666667 ft
Pressure Drop	2.127718891 psi
<b>Tube Side</b>	
Flow area per tube $A_F$	0.594 inch <sup>2</sup> /tube
$A_T$	0.3856875 inch <sup>2</sup>
Mass Velocity $G_T$	170752.2282 lb/hr.ft <sup>2</sup>
Equivalent Diameter $D_e$	0.0725 Ft
Viscosity $\mu$	1.7424 lb/ft.h
Reynolds Number Re	7104.876344
$J_H$ Factor	35
K	0.14
( $cp \times u/k$ )	2.086640163 BTU/hr.ft <sup>2</sup> .(°F/ft)
$H_i$	141.0280 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
f	0.00027
SG	0.826
Pressure Drop	0.402928465 psi

The heat exchanger E – 202 hot fluid mass flow rate 65857 lb/h, specific heat capacity 0.4386 BTU/lb.°F, overall heat transfer co-efficient 145 (assuming), inlet temperature 135 °F, outlet temperature 95 °F and Q 2416000 BTU/h. The shell side pass is 2 and internal diameter 21.25 inch. The cold fluid mass flow rate 123420 lb/h, specific heat capacity 1.0303, overall heat transfer co-efficient 145 (assuming), inlet temperature 81 °F and outlet temperature 100 °F. The tube side 52 BWG 1 inch, length 16 ft, internal diameter 0.62 inches, outer diameter 0.75 inches and passes 4. Table 21 shows the operating and designing parameter heat exchanger E – 202.

Hot Fluid °F	Temperature °F	Cold Fluid °F	Difference °F
135	Higher	100	35
95	Lower	81	14
40	Differences	19	21

Table 21. Operating and designing parameter heat exchanger E – 202

Parameters	Calculated
LMTD $T_M$	22.91849003 °F
R	2.105263158
S	0.351851852
$F_T$	0.93
$\Delta t$	21.31419572 °F

Area (A)	781.7357587 ft <sup>2</sup>
Number of tubes N <sub>T</sub>	248.8970194
<b>Calculation of U<sub>D</sub></b>	
Shell ID	21.25 inch
Pitch	1.0" square pitch
Number of Tubes	246
U <sub>D</sub>	146.7076 BTU/hr.ft <sup>2</sup> .°F
<b>Shell Side</b>	
Baffle Spacing B	4.25 inches
Flow Area A <sub>F</sub>	0.156792535 ft <sup>2</sup>
Mass Velocity G	420026.3751 lb/hr.ft <sup>2</sup>
Equivalent Diameter De	0.079166667 ft
Viscosity μ	1.02003 lb/ft.h
Reynolds Number Re	32599.1275
J <sub>H</sub> Factor	110
K	0.083
(cp×u/k)	1.75335 BTU/hr.ft <sup>2</sup> .(°F/ft)
h <sub>o</sub>	202.20705 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
F	0.0016
SG	0.563
Number of Crosses	45.17647059
D <sub>s</sub>	1.770833333 ft
Pressure Drop	9.706034644 psi
<b>Tube Side</b>	
Flow area per tube A <sub>F</sub>	0.302 inch <sup>2</sup> /tube
A <sub>T</sub>	0.12897917 inch <sup>2</sup>
Mass Velocity G <sub>T</sub>	956894.847 lb/hr.ft <sup>2</sup>
Equivalent Diameter D <sub>e</sub>	0.051666667 Ft
Viscosity μ	1.7424 lb/ft.h
Reynolds Number Re	28374.4072
J <sub>H</sub> Factor	90
K	0.36
(cp×u/k)	1.7085 BTU/hr.ft <sup>2</sup> .(°F/ft)
H <sub>i</sub>	1071.36533 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
f	0.00027
SG	1
Pressure Drop	4.78024483 psi

The heat exchanger E – 207 hot fluid mass flow rate 38966 lb/h, specific heat capacity 0.46 BTU/lb.°F, overall heat transfer co-efficient 73 (assuming), inlet temperature 145 °F, outlet temperature 100 °F and Q 1100000 BTU/h. The shell side pass is 1 and the internal diameter 19.25 inch. The cold fluid mass flow rate 41203 lb/h, specific heat capacity 1.0303, overall heat transfer co-efficient 73 (assuming), inlet temperature 81 °F and outlet temperature 100 °F. The tube side 52 BWG 1 inch, length 16 ft, internal diameter 0.62 inches, outer diameter 0.75 inches and passes 2. Table 22 shows the operating and designing parameter heat exchanger E – 207.

Hot Fluid °F	Temperature °F	Cold Fluid °F	Difference °F
145	Higher	100	45
100	Lower	81	19
45	Differences	19	26

Table 22. Operating and designing parameter heat exchanger E – 207

<b>Parameters</b>	<b>Calculated</b>
LMTD T <sub>M</sub>	30.15459412 °F
R	2.368421053
S	0.296875
F <sub>T</sub>	0.86
Δt	25.93295094 °F
Area (A)	581.0558615 ft <sup>2</sup>
Number of tubes N <sub>T</sub>	185.002503
<b>Calculation of U<sub>D</sub></b>	
Shell ID	19.25 inch
Pitch	1.0" square pitch
Number of Tubes	220
U <sub>D</sub>	61.38719 BTU/hr.ft <sup>2</sup> .°F
<b>Shell Side</b>	
Baffle Spacing B	3.85 inches
Flow Area A <sub>F</sub>	0.128667535 ft <sup>2</sup>

Mass Velocity G	302842.5164 lb/hr.ft <sup>2</sup>
Equivalent Diameter De	0.079166667 ft
Viscosity μ	0.742456 lb/ft.h
Reynolds Number Re	32291.5197
J <sub>H</sub> Factor	100
K	0.07
(cp×u/k)	1.69607 BTU/hr.ft <sup>2</sup> .(°F/ft)
h <sub>o</sub>	149.968 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
F	0.0017
SG	0.88
Number of Crosses	49.87012987
D <sub>s</sub>	1.604166667 ft
Pressure Drop	3.429865316 psi
<b>Tube Side</b>	
Flow area per tube A <sub>F</sub>	0.302 inch <sup>2</sup> /tube
A <sub>T</sub>	0.230694444 inch <sup>2</sup>
Mass Velocity G <sub>T</sub>	178604.2143 lb/hr.ft <sup>2</sup>
Equivalent Diameter D <sub>e</sub>	0.051666667 Ft
Viscosity μ	1.7424 lb/ft.h
Reynolds Number Re	5296.076909
J <sub>H</sub> Factor	17
K	0.36
(cp×u/k)	1.70845 BTU/hr.ft <sup>2</sup> .(°F/ft)
H <sub>i</sub>	202.369 BTU/hr.ft <sup>2</sup> .°F
<b>Pressure Drop</b>	
f	0.0003
SG	1
Pressure Drop	0.113546484 psi

Table 23 summarize important parameters of heat exchanger.

**Flash Drum**

Generally, the purpose of a vessel in unit processing is to either give hold-up time or to make a partition between twofold or multiphase of the blended stream process stream. In this procedure, a Vapor-Liquid separator is utilized. The setup of a vapor/fluid separator relies upon numerous elements. Before making a vessel plan one needs to settle on the configuration of the vessel as for among others direction, sort of feed inlets, kind of heads and simplicity of separation [3, 19].

The size of a vertical Vapor-Liquid separator ought to be managed by the expected flow rate of vapor and fluid from the drum. The sizing methodology depends on the presumptions that those flow rates are known. The vertical vessel ought to be structured with a length to diameter ratio of around 3 to 4, the retention time, as most heuristics predict ought to be in the range of 2 to 10 minutes. The fluid hold up the volume which can be resolved from the maintenance time is then used to compute the high fluid level of the fluid hold up [3].

**a) Maximum allowable velocity**

$$V_{max} = K_t \sqrt{\frac{\rho_1 - \rho_v}{\rho_v}} \tag{21}$$

where; K<sub>t</sub> is the vapor handling capacity rely on the service of the vessel. The separator should be huge to handle the gas flow rate in process conditions.

**b) Settling velocity in a vertical vessel**

The plan of a vertical vapor-fluid separator depends on the terminal settling speed of a fluid bead of determined size, settling affected by gravity. The equation for settling velocity is given by:

$$V_t = \sqrt{\frac{4gD_p(\rho_1 - \rho_v)}{\rho_v}} \tag{22}$$

**c) Cross-sectional area**

Knowing that the flow rate of vapor (Q<sub>g</sub>) that will be leaving the column is determined from the given material balance, the cross-sectional area of the vertical vessel can be calculated as;

$$A_v = \frac{Q_g}{V_m} \tag{23}$$

**d) Diameter**

The diameter is evaluated from the cross-sectional area of the vessel.

$$D_v = \sqrt{\frac{4A_v}{\pi}} \tag{24}$$

**Height of Vessel**

The height of the vessel is calculating by the flow rate of liquid leaving from the bottom of the vessel and the assumed retention time (minutes) of the liquid hold up.

Another assumption is to maintain the liquid hold up level up to one-third of the vessel height.

$$H_v = \frac{(\text{retention time} \times V_l)}{(H_{pool} \times \text{Area of the vessel})} \tag{25}$$

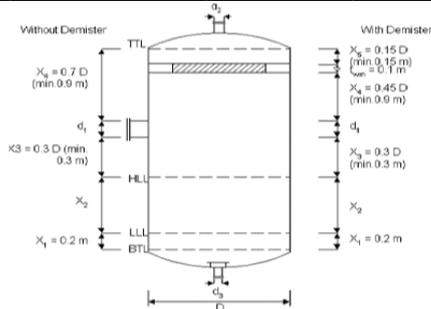
**The volume of Liquid Hold up**

Figure 6 portrays the flash vessel. The volume of liquid hold up ( $V_{pool}$ ) is calculated from the level of liquid hold up as;

$$V_{pool} = \frac{(H_{pool} \times 4)}{\pi \times D_v^2} \tag{26}$$

**Table 23. Important parameters of the heat exchanger**

Exchanger number	Description	Total Area (ft <sup>2</sup> )	Shell Internal Diameter (inches)	Number of tubes (square pitch)	Heat Duty (MMBtu/hr)	Shell side Pressure drops (psi)	Tube side Pressure drops (psi)
E-100	Xylene feed Chiller	789.85	21.25	240	1.64	0.11	1.45
E-101	Filtrate heater (2 <sup>nd</sup> Stage)	163.36	13.25	52	2.50	0.023	2.94
E-102	Filtrate heater (1 <sup>st</sup> Stage)	217.81	13.25	52	0.715	0.009	3.61
E-200	Furnace pre-heater	5698	35	748	45.0	2.12	0.4
E-202	Trim cooler	787.74	21.25	246	2.42	9.71	4.78
E-203	Distillation pre-heater	1249.8	27	408	3.80	1.36	2.26
E-207	Trim cooler	581.1	19.25	220	1.1	3.43	0.1135



**Fig. 6. Flash vessel.**

Table 24 shows the parameter of flash drum.

**Table 24. Parameter of flash drum**

Parameter	Data
Temperature	95 °F
Pressure	140 psig
Design pressure	220 psig
Φ	45°
Density	0.1185 ft <sup>3</sup> /lb
Vapor phase density	0.135 ft <sup>3</sup> /lb
Liquid phase density	7.923 ft <sup>3</sup> /lb
Retention time	2 minutes
K	0.34 ft/s
Particle diameter	300 microns
Gravitational acceleration	32.2 ft/sec <sup>2</sup>
Vapor flow rate	18,300 lb/hr

Volumetric flow rate =  $Q = 42.8973 \text{ ft}^3/\text{s}$

Terminal Velocity =  $U_t = 1.56114 \text{ fps} = 2 \text{ fps}$

Settling velocity =  $U_s = U_t = 2 \text{ fps}$

Maximum allowable velocity =  $V_{allowable} = 2.58241 \text{ fps}$

Cross-sectional area of vessel =  $A_v = 16.6114 \text{ ft}^2$

Diameter of vessel =  $D_v = 4.59864 \text{ ft}$

Length of vessel =  $L_v = 15.1958 \text{ ft}$

Length to Diameter ratio =  $L/D = 3.30441$

**Liquid hold up volume**

Mass flow rate of liquid = 40110 lb/hr

Molecular weight of stream = 104.8 lbmol/lb

Density of liquid stream = 15.89 lb/ft<sup>3</sup>

Height of liquid hold up section = 5.0652662 ft

Volume of liquid pool = 84.140969 ft<sup>3</sup>

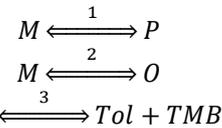
Total volume of tank =  $V_t = 252.423 \text{ ft}^3$

**Table 25. Result card for vertical flash drum**

Parameters	Values
Retention time	2 min
Liquid flow rate	40110 lb/hr
Vapor flow rate	18300 lb/hr
Diameter	4.6 ft
Length	15.1 ft
Settling velocity	2 ft/sec
L/D ratio	3.3

**Reactor design**

The reactor used in the isomerization process is a packed bed reactor; the packed bed reactor differs in the procedure of its designing. Dealing with membrane reactors, packed bed reactors or cases of gas-phase reactions are complex. In such cases, it is more convenient and efficient that the reaction rate equations are expressed as the molar flow rates instead of conversion, where just one equation is involved. Cases of gas-phase reaction involve multiple reactions most of the time and requirement of more than just one equation is felt. For the reason since isomerization of p-xylene is also a complex gas-phase reaction requiring a packed bed reactor reaction the designing of its major unit operation would be followed in the sequence mentioned below [6, 16].



The gas phase pressure drop in terms of molar flow rates;

$$\frac{dP}{dW} = - \frac{\beta_0}{Ac * (1 - \Phi) * \rho c} \frac{P_o F_T}{P F_{Ti}} \tag{27}$$

$$\frac{dF_M}{dW} = - \frac{C_{T0} P}{F_T P_o} [K_1 F_M + K_2 F_M + C_{T0} \frac{F_M^2 P}{F_T P_o} K_3 - K_{-1} F_P - K_{-2} F_O] \tag{28}$$

$$\frac{dF_P}{dW} = - \frac{C_{T0} P}{F_T P_o} [K_1 F_M - K_{-1} F_P] \tag{29}$$

$$\frac{dF_O}{dW} = - \frac{C_{T0} P}{F_T P_o} [K_2 F_M - K_{-2} F_O] \tag{30}$$

$$\frac{dF_{TOL}}{dW} = C_{T0} \frac{2 F_M^2 P^2}{F_T^2 P_o^2} \cdot K_3 \tag{31}$$

$$\frac{dF_{TMB}}{dW} = C_{T0} \frac{2 F_M^2 P^2}{F_T^2 P_o^2} \cdot K_3 \tag{32}$$

$$F_T = F_M + F_O + F_P + F_{TOL} + F_{TMB} + F_I$$

Using Poly-math to get this ordinary differential equation

solved.

$$\frac{d(Fm)}{d(W)} = - \left( \frac{Cto * P}{Ft * Po} \right) * (Fm * K1 + Fm * K2 + K3 * \left( \left( \frac{Cto * Fm^2}{Ft * Po} \right) - Fp * K_{-1} - Fo * K_{-2} \right)) \quad (33)$$

$$\frac{d(Fp)}{d(W)} = - \left( \frac{Cto * P}{Ft * Po} \right) * (Fm * K1 - Fp * K_{-1}) \quad (34)$$

$$\frac{d(Fo)}{d(W)} = - \left( \frac{Cto * P}{Ft * Po} \right) * (Fm * K2 - Fo * K_{-2}) \quad (35)$$

$$\frac{d(Ftol)}{d(W)} = 0.5 * \left( \frac{Cto * Fm * P}{Ft * Po} \right)^2 * K3 \quad (36)$$

$$\frac{d(Ftmb)}{d(W)} = 0.5 * \left( \frac{Cto * Fm * P}{Ft * Po} \right)^2 * K3 \quad (37)$$

$$\frac{d(P)}{d(W)} = -0.00013 * \frac{Po * Ft}{P * Fto} \quad (38)$$

Differential equation key: Equation 28 = equation 33, Equation 29 = equation 34, Equation 30 = equation 35, Equation 31 = equation 36, Equation 32 = equation 37,

Equation 27 = equation 38.

Catalyst bed diameter = 7 ft = 2.134146341 m

Mass flow rate = 65857 lb<sub>m</sub>/h = 29935 kg/h

Density of gas stream = 0.19 lb<sub>m</sub>/ft<sup>3</sup> = 3.047561309 kg/m<sup>3</sup>

D<sub>p</sub> = 0.25 in = 0.020833333 ft, Φ = 0.45,

G<sub>c</sub> = 4.17E+08 lb<sub>m</sub>.ft/(lb<sub>f</sub>.h)

1-Φ = 0.55

ρ<sub>c</sub> = 753 kg/m<sup>3</sup> = 46.94573316 lb/ft<sup>3</sup>

W = 13500 lb = 6136.363636 kg

A<sub>c</sub> = 38.465 ft<sup>2</sup> = 3.575345776 m<sup>2</sup>

G = 1712.127908 lb<sub>m</sub>/ft<sup>2</sup>.h = 8372.616768 kg/m<sup>2</sup>.h

β<sub>o</sub> = 18.7580285 lb<sub>f</sub>/ft<sup>3</sup> = 2.942468996 KPa/m

β<sub>o</sub>/(A<sub>c</sub>×(1-Φ)×ρ<sub>c</sub>) = 0.000131043 psi/lb

ρ<sub>b</sub> = 25.82015324 lb/ft<sup>3</sup> = 414.15 kg/m<sup>3</sup>

L = 13.59280906 ft = 4.144149104 m

K<sub>1</sub> = 4.38 m<sup>3</sup>/kg.cat.h = 70.25430807 ft<sup>3</sup>/lb.cat.h

K<sub>2</sub> = 2.2 m<sup>3</sup>/kg.cat.h = 35.287552 ft<sup>3</sup>/lb.cat.h

K<sub>3</sub> = 31.81 m<sup>6</sup>/kg.mole.kg.cat.h = 18004.62377

ft<sup>6</sup>/lbmol.lb.cat.h

K<sub>-1</sub> = 0.38 m<sup>3</sup>/kg.cat.h = 6.095122618 ft<sup>3</sup>/lb.cat.h

K<sub>-2</sub> = 0.19 m<sup>3</sup>/kg.cat.h = 3.047561309 ft<sup>3</sup>/lb.cat.h

Table 26. Result of ODE solution by Polymath

Sr. No.	Variable	Initial value	Minimal value	Maximal value	Final value
1	Cto	0.0011	0.0011	0.0011	0.0011
2	Fi	4014.7	4014.7	4014.7	4014.7
3	Fm	298.	211.387	298.	211.387
4	Fo	23.	23.	52.0717	52.0717
5	Fp	86.	86.	142.587	142.587
6	Ft	4424.	4424.	4424.	4424.
7	Ftmb	0	0	0.4771247	0.4771247
8	Fto	4424.	4424.	4424.	4424.
9	Ftol	2.3	2.3	2.777125	2.777125
10	K1	70.	70.	70.	70.
11	K2	35.	35.	35.	35.
12	K3	1.8E+04	1.8E+04	1.8E+04	1.8E+04
13	K <sub>-1</sub>	6.	6.	6.	6.
14	K <sub>-2</sub>	3.	3.	3.	3.
15	P	175.	173.2361	175.	173.2361
16	Po	175.	175.	175.	175.
17	W	0	0	1.35E+04	1.35E+04

Conversion m-xylene obtained:

$$X = (Fm_o - Fm) / Fm_o$$

$$X = (298 - 211) / 298 = 29.9\%$$

Pressure drop calculation Ergun equation in terms weight of the catalyst.

$$dp/dw = (-\beta P_o F_T) / [A_c * (1-\Phi) * \rho_c P_{TI}]$$

$$\Delta P = P_o - P = 175 - 173.5 = 1.5 \text{psi}$$

### Furnace

Furnaces are a flexible class of hardware where heat is freed and moved directly or in a circuitously to a liquid mass to impact a chemical or physical change. Combustion furnaces are of two general types, fired heaters and converters. Fired heaters are furnaces that produce heat because of the burning of the fuel. The heat freed is moved to the material to be heated directly or by implication (fired - tube boiler and tubular heater). In tubular or pipe-still warmers process liquid streaming inside tubes mounted inside the furnace are heated by gases delivered by the ignition of fluid or vaporous fuel. These heaters are broadly utilized for warming purposes in oil refining, petrochemical plants, and other industries. Tubular fired heaters are commonly worked with two segments; a radiant segment, called firebox, and a convection area pursued by the stack. The hot vent gases emerging in the radiation segment

stream next into the convection segment where they circulate at rapid over the tube bank before leaving the heater from the stack [17].

A third segment, known as the shielding segment, isolates the radiation segment from the convection area. It comprises of a few lines of exposed tubes which shields the convective cylinders from direct radiations. Fired heaters are generally named vertical cylindrical or box-type heaters relying on the geometrical arrangement of the radiant area. In box-type warmers, the radiant area has commonly square cross-segment. Box type heaters are most appropriate for enormous limits and huge warmth obligations. This makes such heaters especially reasonable for topping units where it is conceivable to expand tube length in both the radiation and convection areas. Generally, around 45-55% of the total heat discharge in the furnace is moved to the procedure liquid in the radiation area, leaving around 25-45% of the rest of the warmth that is being moved either in convection segment or being diverted by flue gasses from the stack. To increase the heat transfer region and in this manner further increment the general productivity of the

radiator, finned or studded cylinders are typically utilized in convection segment. By this implies it is regularly conceivable to accomplish the normal transition in the convection area equivalent to that in the radiation segment. Lobo and Evans have made a complete study of petroleum heaters and the Wilson, Lobo and Hottel radiation equation [14].

$$R = \frac{1}{1 + \frac{g \sqrt{\frac{Q}{\alpha A_{cp}}}}{4200}} \tag{29}$$

They also present a theoretical equation that appears to check well with all types and arrangements of heaters. In the convection region heat is transferred both by convection and radiation.

Q = 9634217 Btu/hr, Number of tubes = 32, A = 25.1183333 ft<sup>2</sup>, Assumed Flux = 11500 Btu/hr.ft<sup>2</sup>, Air Fuel Ratio = 22.5 lbmol/lbmol, T<sub>g</sub> = 1600 °F, T<sub>s</sub> = 1000 °F, A<sub>cp</sub> = 533.3333 ft<sup>2</sup>, αA<sub>cp</sub> = 469.3304 ft<sup>2</sup>, Assume: H = 20 Ft, B = 16 Ft, L = 10 Ft.

L: B: H = 10/10: 20/10: 50/10

Approximate; L: B: H = 1:2:2

Mean length calculation: L = 14.36289793, h = 50 ft

P (CO<sub>2</sub> + H<sub>2</sub>O) = 0.22 atm

P<sub>L</sub> = 3.3 atm.ft, T<sub>s</sub> = 1000 °F, T<sub>g</sub> = 1600 °F

P<sub>F</sub> = 0.48

T<sub>g</sub> determined = 15500 °F, Pseudo temperature = 3400 °F,

Air pre-heat temperature = 400 °F, R = 0.5454

q = 11500 Btu/hr.ft<sup>2</sup>

**Distillation unit (Light aromatics column)**

The distillation segment contains one feed stream and two item streams. The feed contains a mole percent of the light part, Z<sub>F</sub>. The product stream leaving the top has a composition of X<sub>D</sub> of the light part. The product stream leaving the base contains creation of X<sub>B</sub> of the light segment. The segment is broken in two areas. The top

segment is alluded to as the rectifying area. The base segment is known as the stripping area. The top item stream goes through a total condenser. This adequately gathers the majority of the vapor distillate to the fluid. The base product stream utilizes a fractional re-boiler. This takes into consideration the contribution of vitality into this section. The purpose of a distillation column is to make use of the relative volatility of a mixture of components and effectively separate them. The purpose of a distillation column in this project study is the separation of lighter ends resulting from the liquid discharge of the flash vessel, so that a relatively pure feed of xylenes is recovered with increased mole percent para-xylene compared to the initial charge of the isomerization plant.

Lewis and Matheson method of calculating the number of ideal plates for a necessary given separation can be used to find the number of plates. An already designed distillation column with 29 plates has been simulated on HYSYS to obtain results for the distillate, bottoms product and off-gases as a result of cold reflux from the condenser [13, 20]. It is further deduced that the following top operating line equations hold for the case of multi-component distillation to give a bottoms product of desired specifications with a reflux ratio of 15. The equations shown are for more relevant components that are meta-xylene, para-xylene and ortho-xylene [21].

$$y_n = (L_n * x_{n+1}) / V_n + (D * x_D) / V_n$$

$$y_{nm} = 0.9375 * x_{n+1} + 0.0269$$

$$y_{np} = 0.9375 * x_{n+1} + 0.0189$$

$$y_{no} = 0.9375 * x_{n+1} + 0.002$$

Furthermore bottom operating lines for the same components follow;

$$y_m = (L_m * x_{m+1}) / V_m + (B * x_B) / V_m$$

$$y_{mm} = 2.089 * x_{m+1} + 0.527$$

$$y_{mp} = 2.089 * x_{m+1} + 0.3517$$

$$y_{mo} = 2.089 * x_{m+1} + 0.1338$$

**Table 27. Result card of distillation column**

Physical Properties	Unit	Reflux	Bottoms	Feed	Distillate	Off Gases
Vapor Fraction		0	0	0.019084	0	1
Temperature	F	196.048427	331.32991	267.999994	196.048427	196.048427
Pressure	psia	20.696	28.696	28.696	20.696	20.696
Molar Flow	lbmole/hr	453.002565	410.455152	440.655	23.199963	6.999885
Mass Flow	lb/hr	47370.99786	43576.19362	46201.8754	2426.046783	199.634999
Liquid Volume Flow	barrel/day	3741.873581	3436.72031	3656.499903	191.635405	28.144188

**Pumps**

A pump is a device that moves liquids (fluids or gases) or slurries, by mechanical activity. Pumps work by some component (ordinarily responding or rotary), and devour vitality to perform mechanical work by moving the liquid. Pumps work through numerous vitality sources, including manual activity, power, motors, or wind control, come in numerous sizes, from a minute for use in medicinal applications to huge modern pumps [9, 20].

**Table 28. Result card for pumps**

Parameter	Octafiner Charge	P-201
Mass flow rate (lb/hr)	46895	16540
Mass flow rate (kg/hr)	21316	36390
Density (kg/m <sup>3</sup> )	868	880
Required volumetric flow rate (m <sup>3</sup> /hr)	24.558	18.795
Differential pressure (psi)	280	50
Differential pressure (KPa)	1930	344.7
Horsepower (KW)	13.116	1.8
Horsepower (HP)	17.655	2.413
Efficiency	54.818	51.436
Brake-Horse power (HP)	32.2	4.692

Mechanical pumps serve in a wide scope of uses, for example, pumping water from wells, aquarium sifting, lake separating and aeration, in the vehicle business for water-cooling and fuel infusion, in the vitality business for pumping oil and gaseous petrol or for operating cooling towers. To cost of utilities pump designing has been studied but limited to the calculation of horse-power required and the break-horse power of the two pumps from the isomerization unit [4, 16].

**Conclusion**

The use of ZSM-5 zeolite catalyst increases the selectivity and probability of isomerization reaction. The modification in the shape of Zeolite catalyst increases the diffusion of paraxylene which is greater than meta and ortho-xylene. Hence preventing diffusion in ZSM-5 pores by lessening the channel size can in all probability lead to increase in isomerization selectivity over the massive disproportionation reaction and furthermore in para-xylene selectivity over ortho-xylene.

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