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**Improvement of the p-xylene and benzene production process
through the disproportionation of the toluene**

**Mejora de la producción de p-xileno y benceno
mediante la desproporción del tolueno**

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REPORT

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1. SUMMARY

This document contains the extension of the thesis carried out during the degree which consisted of the design of a plant to obtain p-xylene and benzene by disproportionation reaction of the toluene that is present in the bottom stream of the hydrocarbon column that is currently sent to the gasoline blend.

The expansion of the work consists of the purification of the xylene mixture and maximization of the production of p-xylene, as well as the realization of elements not designed during the reference project.

The new unit starts with the modification of the xylene separation column in which previously p-xylene and m-xylene were obtained by means of a 132-tray distillation column, now separating the heavy aromatics from the rest.

The stream containing the xylenes is sent to the continuous adsorption column, using hydrated Y-type zeolite as adsorbent, the physisorption is carried out by means of SMB technology, simulated moving bed technology. The stream rich in p-xylene which is separated by means of a distillation column obtaining the product, the desorbent is obtained which is recirculated to the adsorption chamber. The stream that does not contain p-xylene is sent to the desorbent recovery zone and the desorbent-free stream is sent to the reaction zone where the isomerization of the xylenes and the dealkylation of the ethylbenzene is carried out in order to obtain benzene at 10 bar and 420 °C. The output stream from the isomerization unit is sent to the benzene separation zone and then sent back to the adsorption column.

Once the process and equipment had been designed, the corresponding P&IDs were drawn up together with the list of pipes. Finally, in order to check the feasibility of the project and its possible implementation, an economic study was carried out.

To carry out the process, an initial investment of 108 M€ is required. Considering the current market, assuming that the price of raw materials, products and their demand remains constant and, a IRR of 21.1 % and a NVP of 25.2 M€ are obtained in a period of 5 years. In addition, the payback of the process is 3 years.

2. INTRODUCTION

This chapter describes the project to contextualize the work. Specifically, it describes what was done in the reference project to know the scope of the project.

Including the study of the technologies present for this application, which is used to define the objectives of this project.

2.1. Reference project

The project presented in this memory is the continuation of the reference work ¹, it should be noted that the project in question is the thesis carried out during the Chemical Engineering degree, in which the first sections of the production process of p-xylene and benzene by means of the disproportionation of toluene are presented.

Figure 1 shows a block diagram of the production process of the previous project in which the equipment was characterized, the P&ID's were designed, the list of instruments, valves and pipes was made, as well as the safety concept of the process, and finally the feasibility of the designed sections and their possible implementation was checked by carrying out an economic analysis.

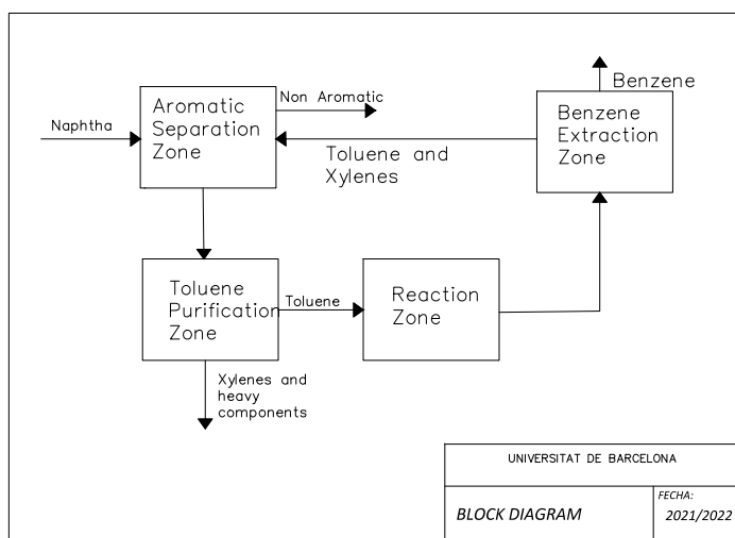


Figure 1 Preliminary block diagram of the production process.

The block diagram consisted of 4 parts, the first one being the separation zone where the aromatic hydrocarbons are separated from the non-aromatics. The aromatics stream containing mainly toluene, xylene and heavy aromatics are separated in the purification zone where a toluene stream is obtained and sent to the reaction zone and

a xylenes stream is obtained for storage for future treatment. The toluene stream then enters the reaction zone where it is disproportionated to obtain benzene and p-xylene. The output stream is sent to the benzene separation zone to obtain a stream of pure benzene, sending the xylene obtained and the unreacted toluene to the purification zone.

2.2. Scope of the project

Once the reference project has been introduced and taking into account that the design did not obtain the desired purity for p-xylene.

The scope of this project is to carry out the design of the p-xylene purification unit, as well as to finish the design of the equipment not carried out in the reference project and to design the process in an optimized manner.

2.3. Preliminary stage

It is necessary to carry out a preliminary stage where the main reasons why the design of this process unit is required are observed, in addition to carrying out a study of the technologies for development.

2.3.1. Product

To understand why a p-xylene purification unit needs to be set up, it is necessary to understand the product and its current market.

Xylene is a colourless liquid that occurs naturally in petroleum. There are three isomers of xylene, depending on the location of the methyl groups on the benzene ring: ortho-xylene (1,2-dimethylbenzene), meta-xylene (1,3-dimethylbenzene) and para-xylene (1,4-dimethylbenzene). These have a high-octane rating, which makes their use in fuels very attractive.

The increase in demand for p-xylene is not due to its use in fossil fuels, but to its use in the production of PET or polyethylene terephthalate, which is a type of plastic polymer widely used for food packaging and textile fibres²

PET is a polymer obtained from a polycondensation reaction between terephthalic acid and ethylene glycol. The p-xylene plays a key role in the production of terephthalic acid, as this is achieved by catalytic oxidation of p-xylene in an acidic medium.

2.3.2. P-xylene market

Global demand for p-xylene is equivalent to 86% of the demand for blended xylenes.³ Over the past 10 years, overall p-xylene capacity has grown considerably globally; however, p-xylene industries experienced vastly contrasting growth in Asia and the Middle East adding new production capacity, while other regions such as North America and Western Europe underwent consolidation of existing units, leading to an increasing density of p-xylene production in the Asian region market.

The market was affected by the COVID-19 pandemic in 2020. As purified terephthalic acid, widely used in the automotive industry, negatively affected the market by temporarily shutting down manufacturing. However, increased use in face shields, clear masks, food, and e-commerce packaging meant that the market was not as affected as para-xylene derivatives, such as purified terephthalic acid itself, dimethyl terephthalate and polyethylene terephthalate, were needed. Once the COVID-19 pandemic was stabilized and car manufacturing returned, the demand for p-xylene was on the rise.⁴

To put the above into numbers, the p-xylene market was estimated at over 50 million tons in 2021 and is expected to register a CAGR, Compound Annual Growth Rate, of over 5 % during the forecast period (2022-2026), as shown in Figure 2.⁵

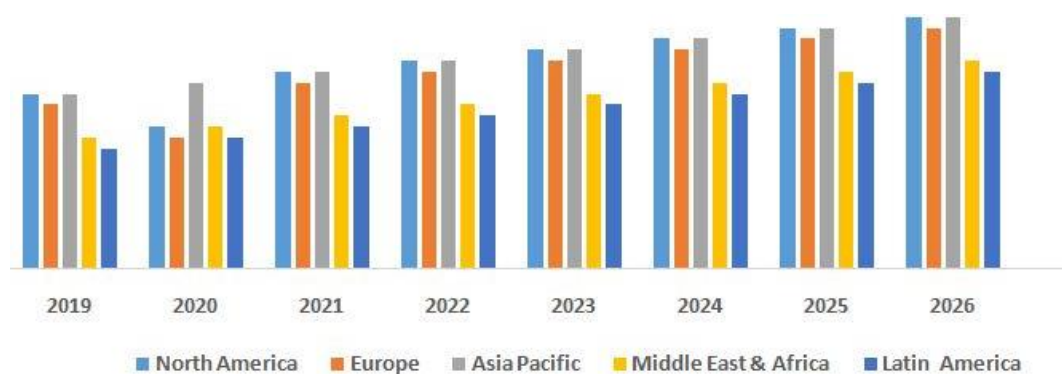


Figure 2. Evolution of p-xylene demand.

(Image extracted from ref. 5)

2.3.3. Study of technologies

The sources used to produce p-xylene are usually composed of a mixture of xylene and ethylbenzene isomers. The separation of the p-xylene isomer from the mixture is a common industrial concern.

Fractional distillation, the most widely used separation method, could be applied with a high number of trays and reflux for the separation of o-xylene and even ethylbenzene, but not for the separation of p-xylene from m-xylene, because their boiling point is too close, so at industrial level, they have had to use different properties of the compounds to achieve the separation of p-xylene, such as their freezing point or their chemical structure for the use of adsorption.

At industrial level, there are three methods for obtaining high purity p-xylene: crystallization, adsorption, or the use of a hybrid process.

A study of the three separation technologies is carried out to select the most suitable one.^{6,7}

Crystallization separation

The crystallization process uses the freezing point of the substances in order to separate them. Crystallization in the p-xylene production process is carried out to solidify the p-xylene from the mixture of isomers because of the isomers present in the stream, p-xylene is the compound with the highest freezing point.

The technology used for the separation by crystallization consists of a stepwise crystallization at different temperatures (3 °C and - 4 °C) and a separation of the crystals generated by using a centrifuge.

In the specific case of p-xylene separation, the maximum recovery of p-xylene is limited by the eutectic point, that is, the temperature point at which a second component starts to crystallize. Typical recovery values are in the range of 60 to 65 % by weight for feed streams with 20 % by weight of p-xylene.⁸

It should be noted that in the crystallization process the control of temperature and cooling rate is key to the size of the crystals.

Currently, the only supplier of this technology on the market is LUMMUS with the update and improvement of a process that was marketed and widely used in the 1970s,

the Chevron process, which used crystallization and centrifuge cycles to achieve a p-xylene purification of more than 99 %.⁹

In 1970, more technologies were commercialized, such as the Amoco and Krupp processes, among others.

Adsorption separation

The adsorption separation technology was launched for the first time in 1961. Since then, the adsorption process has always used the same operating principle, only improvements have been made to the catalyst or desorbent for better recovery and purification.¹⁰

The separation by adsorption consists of using a solid bed of zeolites, specifically Ba-exchanged faujasite-type Zeolite hydrated, where the only compound with the capacity to enter to the pores of the zeolites is the p-xylene, once the product mixture has passed through the column it is rinsed with the desorbent that is capable of washing the bed and extracting the p-xylene from the zeolites, in this process there is a physisorption in the selective centers of the particle.

After this, the wash stream is taken to a distillation column to separate the product, p-xylene, from the desorbent that will re-enter the column obtaining a purity higher than 99.3 %wt. and a total recovery higher than 90 %.

Hybrid process separation

Hybrid processes use the union of the two technologies, simplifying the adsorption column and reducing the volume of the equipment.

This technology is used in existing crystallization production processes in order to increase production and recovery of p-xylene.

Selection of technology

Once the 3 technologies for the purification of p-xylene are known, it is intended to give the reasons for the selection of the technology.

At present, there is a moderate percentage of production processes where the purification of p-xylene is carried out by crystallization, this is due to the fact that the adsorption process began to be commercialized in 1961. Another point is that before the 1970s there were many companies that commercialized crystallization, despite the fact that it was a process that required many stages and an average p-xylene recovery of 70 % was generally obtained, as well as requiring a high amount of energy and exhaustive control of the process variables, since the kinetics of crystallization can influence the purity of p-xylene, as the crystals must have a size of 0.5 mm for optimum separation.

After the 1970s, the first adsorption-based plants were built, not only because of their high recovery and purity, but also because adsorption technology has a lower cost in terms of equipment.

Therefore, the choice of technology for the framework of the project is straightforward, with adsorption being the direct choice.

Within the adsorption production process, there are different companies that commercialize it, each including different variants within the same process, such as the Parex unit from UOP and the *Eluxyl* unit from Axens. Both cases would be valid for the development of the project, but due to its age, the UOP Parex unit is more documented.

PAREX Technology

One of the easiest ways to understand PAREX technology and how it is described in the literature is to make the analogy with a batch elution chromatography where a mixture of two compounds A (product) and B (other compounds) have different affinity to the adsorbent on the column.¹⁰

Separation of A and B by elution chromatography is performed by injecting a pulse of the mixture, in most cases diluted in a suitable solvent, and then reading the pulse with pure solvent. Since component A has a higher affinity for the adsorbent than component B, component A will migrate along the column at a slower rate than component B. If the chromatographic column is long enough, both A and B can be collected pure at the

downstream end of the column, but at different times. For proper operation of this separation, it is always necessary to regulate the frequency and duration of the pulse and the flow rate, where separation may not be obtained if the two peaks overlap. The main problem with this separation is that both component A and component B are obtained at the same point in the system, and it is a batch feed.

To remove this problem, if the solid were to move continuously in the opposite direction to the liquid phase and with a velocity greater than the velocity of the concentration front of A and less than the velocity of the concentration front of B, then both solutes can be separated continuously. B would be obtained at the bottom of the column, and A would be obtained with the solid at the head, as shown in Figure 3.

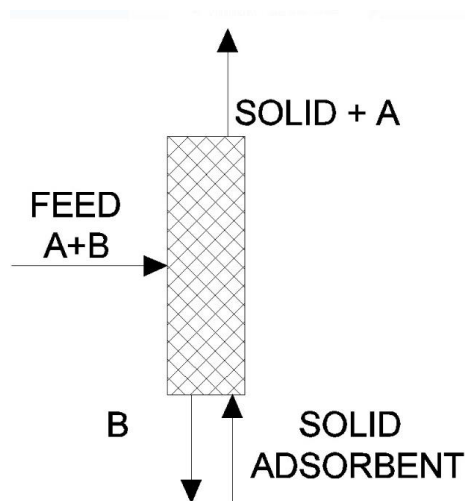


Figure 3. Simplified schematic of the PAREX Column's operating principle.

The industrial use of the operating principle explained in the previous point is the so-called TMB, True Moving Bed, which consists of a train of 4 adsorption columns in countercurrent and connected to each other, where the liquid moves between the different columns just like the solid, but in opposite direction with two inlets, feed and desorbent, and two outlets, extract and refined.

The main problem with the application of the principle described by the TMB technology comes from the movement of the solid in the column as this is not practical as it generates an erosion of the equipment, wear and fractionation of the adsorbent

particles due to friction with the solid and between them, and an impossible operation of the equipment as it is extremely difficult to guarantee a constant movement of the solid and a piston flow inside the column, making the separation impossible.¹¹

In order to eliminate the difficulties described in the TMB working principle, the SMB, simulated moving bed, was developed. In the SMB, the solid is stationary and its movement is simulated by changing the positions of the four ports periodically and synchronously in the direction of the fluid flow.

When explaining the TMB theory it has been described that there are a total of 4 columns and as in the SMB in a different way 4 zones can be described:

ZONE I: This zone is located between the feed and the refining extraction port, where the desired compound is adsorbed and does not reach the refining port. **Adsorption zone.**

ZONE II: This zone is located between the extract zone and the feed, this zone has the function that the adsorbed compound in smaller quantities does not contaminate the extract stream, the adsorbed compound stream. **Purification zone.**

ZONE III: It is located between the extract port and the desorbent inlet. In this zone, the desorbent that enters pure, displaces the adsorbed component from the selective pores and its function is to regenerate the adsorbent and prevent the most adsorbed species from reaching the next zone. **Desorption zone.**

ZONE IV: It is located between the exit point of the refining and the introduction point of the desorbent, it is a buffer zone between zone I and zone III and its function is to avoid that the desorbent does not arrive totally clean to zone I. **Buffer zone.**

Figure 4 shows the schematic diagram showing the different zones of the PAREX column.¹²

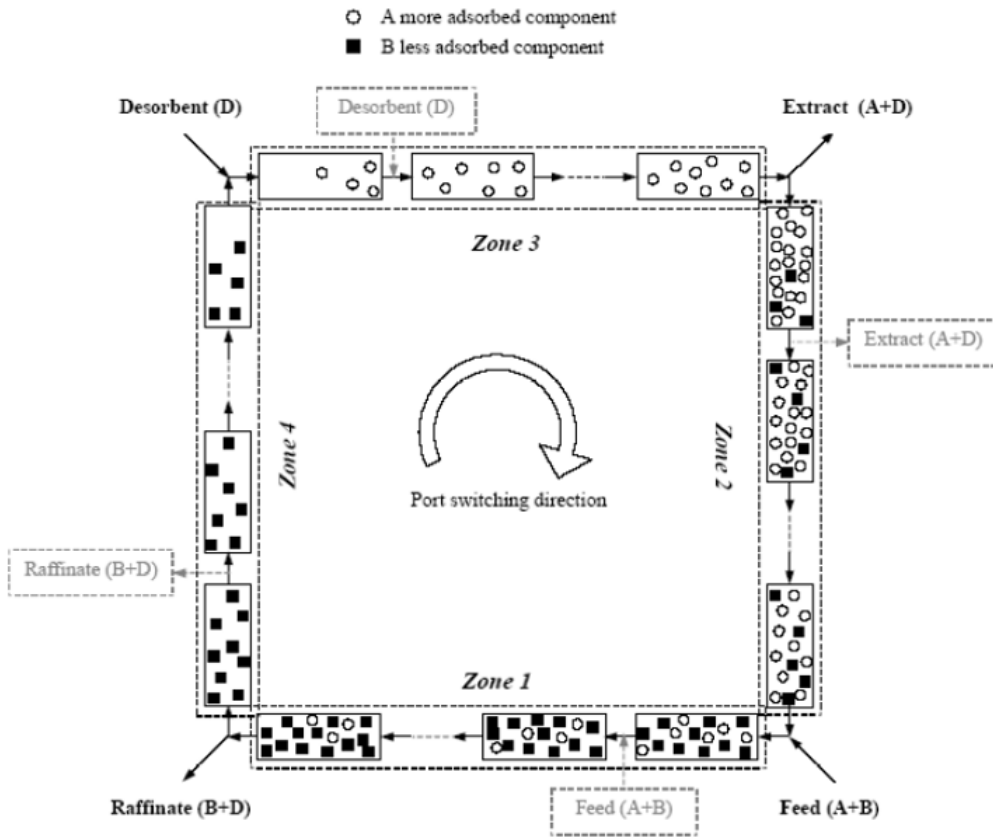


Figure 4 Schematic of SMB technology.

(Image extracted from ref. 12)

3. OBJECTIVES

As stated in the scope of the project, the objective is to design the p-xylene purification unit and obtain p-xylene and benzene by disproportioning the toluene present in the naphtha stream.

Having as main objective the design of the production process to obtain two products, p-xylene with a purity of 99.4 % and a purity for benzene of 99.5 %.

Breaking down the main objective into smaller objectives, the following objectives are included:

- To carry out a study of the technologies present on the market today and their evolution for the purification of p-xylene with respect to its isomers.
- Synthesis of the complete production process.
- Simulation of the different process units for the characterization of the equipment.
- Optimization of the production process.
- To check the feasibility of the project and its possible implementation, the economic study of the project has been carried out.

4. METODOLOGY

To achieve the objectives of the project, the process simulation tool Aspen plus V.12 is used in addition to bibliographic sources that corroborate the different units of the process.

The new equipment is designed together with the simulation of the reference project in order to use the same database and method of calculating the properties. The method used is the UNIFAC¹³, which is a semi-empirical system for predicting the activity of non-electrolytes in non-ideal mixtures. UNIFAC uses the functional groups present in the molecules that make up the liquid mixture to calculate the activity coefficients. Using interactions for each of the functional groups present in the molecules, as well as some binary interaction coefficients by updating terms that have been available over the last two years. Since it was verified during the reference project that it provided reliable data.

The tool will be used to carry out the process design and the characterization of the different process units.

On the other hand, different tools provided by the simulator will be used to optimize the equipment, as well as the option of linking Aspen Plus with Excel.

5. BASIC ENGINEERING

The first step to carry out the basic engineering is to know the bases of the project; these bases are described in the reference project. ¹

5.1. Block diagram

The block diagram of the project shown in Figure 5. consists of 4 new stages. Continuing with the xylenes and heavies stream obtained from the toluene purification is sent to the heavies separation zone, the stream containing the heavies is stored and the stream containing the xylenes is sent to the p-xylene purification zone. In the p-xylene purification zone, two streams are obtained, the stream rich in p-xylene is sent directly to storage as a product and the other stream containing the remainder is sent to the isomerization zone. In the isomerization stage, p-xylene is obtained by equilibration of its isomers and benzene from the dealkylation of ethylbenzene. The output stream from the isomerization unit is sent to the benzene separation zone and the remainder is sent back to the p-xylene purification.

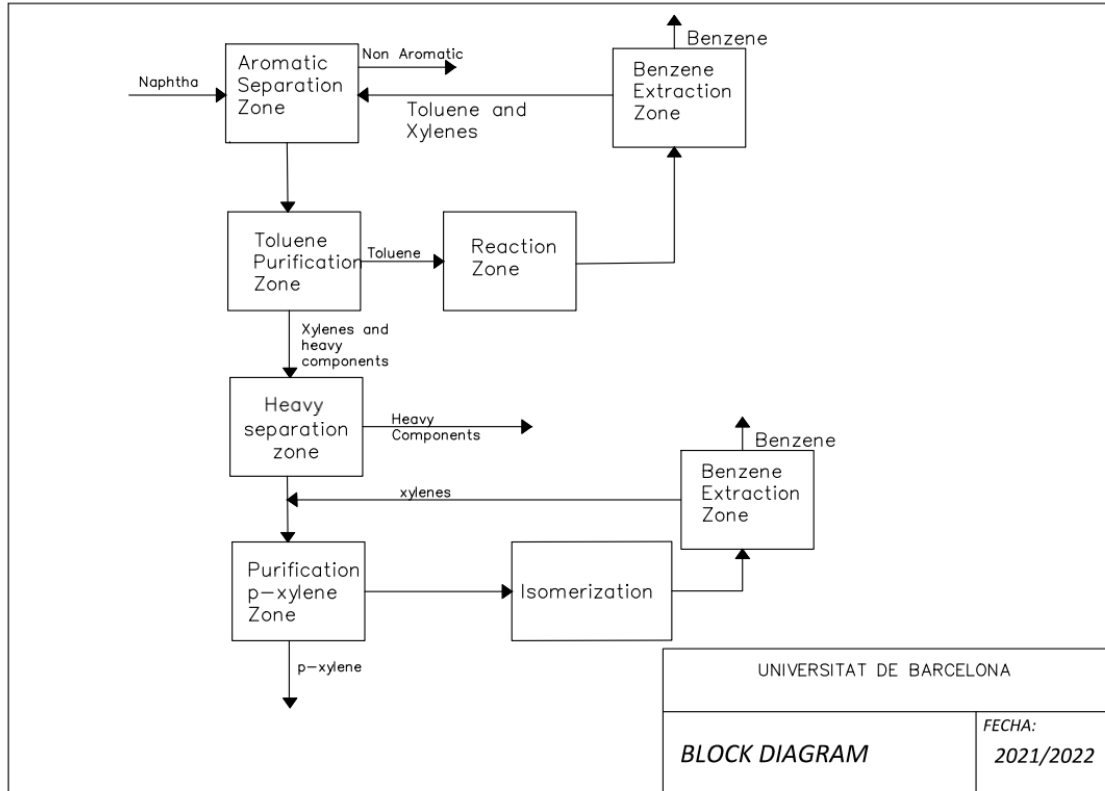


Figure 5. Block diagram of the process.

5.2. PFD

The unit for obtaining p-xylene and benzene from toluene disproportionation starts from the hydrocarbon column bottom stream that is currently sent to gasoline blending. Part of this stream is sent to the newly designed process.

First, the extractive distillation of the hydrocarbons is carried out to separate the aromatic compounds from the non-aromatic ones, using a solvent that is selective for aromatics, N-methyl-2-pyrrolidone. This distillation requires two columns, the extractive distillation column, and the recovery column. The first, T-101, separates the aromatic hydrocarbons from the non-aromatic hydrocarbons and the second, T-201, recovers the solvent, separating it from the aromatic compounds and then recirculating it to the first column.

The T-101 column, which operates at atmospheric pressure, is fed with the solvent at 80 °C and the hydrocarbon stream at 121 °C with a volumetric ratio of solvent/hydrocarbon of 1.5/1. The inlet pressures of both streams (1.15 bar (a) and 1.35 bar (a), respectively) have been defined according to the fact that they have to be at least the pressure of the inlet plate plus a safety margin. Then, the non-aromatic compounds come out of the head of the column and are sent to the petrol blending. On the other hand, at the bottom of the column, the aromatic compounds are mixed with the solvent and introduced into the T-201 column at the pressure and temperature conditions (1.37 bar(a) and 178 °C). In this column, also operated at atmospheric pressure, the pure stream of aromatic hydrocarbons exits at the head, while at the bottom of the column the solvent is recirculated in its entirety back to the T-101 column. This recirculation is at 216°C and must be cooled to the required temperature at the solvent inlet (80 °C). To do this, firstly, a low-pressure steam generator (5.6 bar(a) and 158 °C), E-122, (Kettle type) is applied to take advantage of part of the heat of the current that is cooled to 180 °C. Then, by means of the AE-132 air coolant, the temperature is lowered to 80 °C.

It should be explained that the supply of fresh solvent and the purging of this compound in the recirculation is carried out discontinuously every 15 days, so that the solvent is recirculated in its entirety. The supply of fresh solvent will also be carried out in the

event that the corresponding meters indicate a lack of the compound and/or non-compliance with the solvent/hydrocarbon ratio.

The distillate stream from T-201 and the bottom stream from T-701 enter the distillation column T-301. Both streams are elevated to the desired pressure (1.4 bar (a)).

The purpose of the T-301 is to separate the toluene from the mixture and send it to the reaction zone for disproportionation of the toluene. The operating conditions of the equipment are 1 bar(a) at 115 °C. The stream coming out of the head is condensed in the AE-321 air cooler and subcooled to 7 °C. Subsequently, part of the stream is recirculated to the column and the other part is sent to the reaction zone. The equipment separates toluene with 99.8 % mass purity.

The toluene stream obtained by T-301 column head, the pressure is raised to the operating conditions of the reactor, specifically 31.4 bar g, to this stream is added the hydrogen recycle, because the inclusion of hydrogen as diluent agent in the reactor greatly decreases the coke deposition on the catalyst, where a minimum ratio of 2 moles of hydrogen for each mole of toluene is required.

Once joined, the heat is reused by means of the heat exchanger, E-501, where the heat from the reactor output stream preheats the stream which is then heated in the H-502 furnace to the operating conditions of the reactor, specifically the temperature of 420 °C. The furnace output enters the PFR reactor where the disproportionation of the toluene takes place in the presence of the catalyst, obtaining a conversion of 30 % of the toluene and a high selectivity of p-xylene and benzene.

This stream, after passing through the exchanger, is cooled to the optimum temperature for separation of the hydrogen from the condensates, which is carried out in the D-504. The gases are recirculated, with fresh hydrogen and a small purge. The liquid stream from D-504 is taken to a stabilizer in order to separate the small part of the incondensable that have not been separated and the lighter ones generated in the reaction from the rest. The liquid stream from the stabilizer is taken to the T-601 column in order to obtain pure benzene at the head of the column. The column bottom containing mainly unreacted p-xylene and toluene is recirculated to the T-301 column. The stream leaving the T-301 column bottom is raised to 1.16 bar(a) and sent to the T-701 column. The purpose of T-701 is to separate the xylenes from the mixture. The

operating conditions of the equipment are 1 bar(a) and 138 °C. The stream leaving at the bottom of the column, which contains the C9 mixture, is sent to the tanks. The stream leaving at the head (containing a mixture of ethylbenzene, p-xylene, m-xylene and o-xylene) is condensed in the AE-721 and subcooled by 7 °C. The stream is raised to the operating conditions of the continuous adsorption column 9 bar (a) and 173 °C, sent to the rotary valve VR-851 of the continuous adsorption column, T-801 and T-802, to this same valve is sent the desorbent at the same conditions of the continuous adsorption column, T-801 and T-802, with the desorbent at the same conditions, 1-4 Dimethylbenzene, 9 bar (a) and 173 °C, in the T-801 and T-802 column two streams are obtained, the refining stream, a stream composed of p-xylene and the desorbent, and the extract stream composed of the non-adsorbed compounds and a part of the desorbent.

The extract stream containing mostly p-xylene and desorbent is reduced in pressure by means of a pressure reducing valve and is sent to the column at 159 °C and 1.11 bar(a) at T-1301 where the p-xylene is obtained at the required purity and the desorbent is recovered and recirculated to the adsorption column T-801/T-802.

On the other hand, the refining stream, the stream that composes the rest of the xylenes and ethylbenzene, is reduced in pressure and sent to the operating conditions of the T-901 column, 164 °C and 1.07 bar(a), as in the T-1301 column, the process compounds are separated from the desorbent, to recirculate it.

The stream obtained at the top of the T-901 column is raised to the pressure of the reactor operating conditions, specifically to 11 bar(a), to this stream is added the hydrogen recycle, as in the disproportionation reaction, it is necessary to include hydrogen as a diluent agent, since in the reactor it greatly reduces the deposition of coke on the catalyst. It has been found in the literature that the optimum ratio for the isomerization of xylenes is around 2 moles of hydrogen for each mole of feed. Once bound it is taken to an exchanger, E-1001, where the heat from the reaction zone is reused for preheating before heating to operating conditions in the H-502 oven, specifically to a temperature of 420 °C. The furnace output is taken to the isomerization reactor, where the equilibrium of the xylene isomers and the dealkylation of ethylbenzene into benzene is obtained. The stream after passing through the exchanger,

E-1001, and is cooled in AE-1003 at 32 °C to separate the incondensable from the condensable by D-1004.

The gases are recirculated, with fresh hydrogen and a small purge. The liquid stream of D-1004 is taken to a stabilizer T-1101 in order to separate the small part of incondensable that have not been separated and light gases generated in the reaction from the rest. The liquid stream is sent to the T-1201 column to separate the benzene from the rest of the components, which are recirculated to the stream of the T-701 to carry out the adsorption again. The Figure 6 shows the process diagram and the material balance.

5.3. Piping and instrumentation diagram (P&ID)

The following section shows the P&IDs of the process and explains the continuous process control. Figures 7, 8 and 9 show the P&ID of a distillation column, the adsorption column, and the reaction zone. The others P&ID are shown in Appendix 1.

5.3.1. Distillation Column

The control explanation of the columns of the production process is grouped together using a common criterion for their correct operation. In the explanation the actuated elements or measuring instruments are mentioned with an X, this being the number of the reference equipment.

Feed pressure control

The pressure is measured by the pressure gauges, PIT-X201 and PIT-X202, respectively, and these values are transmitted to the pressure controller with its setpoint and transferred to the variable speed drive of the motors of the corresponding delivery pumps to increase the discharge pressure. In case of a pressure reducer, manipulation of the equipment will be necessary to adjust to the operating conditions.

Control of the top composition

To control the composition of the head, two variables are used. The first one is the pressure, the pressure inside the column is measured by means of the PIT-X203 and PIT-X204 gauges and it is transmitted to the pressure controller with its determined setpoint, transferring it to the power variator of the air coolant motor, AE-X31, condensing in greater or lesser quantity depending on the case. Therefore, if the column pressure increases, the controller will compare this pressure value with the setpoint and tell the air coolant motor drive to increase its value. This will result in increased head vapor condensation and a decrease in column pressure. On the other hand, in the event of a rise in temperature, detected by the TIT-X202 and TIT-X203 temperature gauges, an increase in temperature would cause compounds with a lower volatility than desired to be obtained at the head of the column.

In both cases, manipulating the V-X501 valve that regulates the reflux inlet to the column to establish the desired value, this value always being validated by the FIT-X401,

that is, it will open or close depending on the scenario that arises. In case of a sudden pressure rise in the equipment that V-X501 cannot regulate, the safety valves (PSV 1 and PSV 2) will relieve this pressure. These valves have a tripping pressure of 3.7 kg/cm².

Column level control

It is measured by means of the level sensor LIT-X303 and LIT-X304, it will be possible to observe different situations such as the level being high and flooding the last plate or detecting that the bottom of the column is emptying and therefore there is a low level that endangers the column bottom pump. In both cases it will manipulate the V-X504 valve to adjust the level to the required level.

Temperature control at the bottom

It is measured by the TIT-X205 and TIT-X206 sensors. In the event of a high temperature scenario or a considerable rise in temperature, V-X502 will close in order to send less flow to E-X41, and as a consequence, E-X41 will provide less energy to T-X01 until the required temperature is established. In the opposite case and the temperature drops, V-X502 will open to provide more flow to E-X41 increasing the working temperature.

Control of the reflux accumulator (D-X31)

In the D-X31 storage tank, the pressure, level and temperature are to be monitored. To keep the accumulator pressure constant, it is measured by PIT-3004 and, as for the pressure in the column, the power variator of the air coolant motor, AE-X31, is manipulated, condensing depending on the case. The accumulator level is measured by means of LIT-X301, and in case of a high or low level, V-X501 is used. The temperature is measured by TIT-X204 and, as in the column, the valve V-X501 is manipulated.

Reboiler control (E-X41)

In the kettle reboiler, pressure, temperature and level are controlled in the same way as in the reflux accumulator. To control the pressure, it is measured by PIT-X005 and manipulates both V-X502 to adjust the pressure value of the column, having a low pressure in E-X41 would mean that the pressure of the column is not the desired one, having to manipulate a low pressure in E-X41 as well as in D-X31 and in T-X01. In the

case of temperature, something similar happens with the temperature control at the bottom of the column, which is measured by TIT-X207 and manipulates V-X504, opening the way to a higher or lower vapor inlet. The level is measured by means of LIT-X306, manipulating V-X502 to adjust to the operating conditions, closing in case of a high level until evaporation at the desired level or opening to enter more flow.

5.3.2. Adsorption Column

For the correct function of the operating column and safe operation there are different control loops that describe the process.

Control the Adsorption

or the correct operation of the different zones of the column, it is necessary to control the inlet and outlet flow rates of the column, all of which are measured by the FIT-8401, FIT-8402, FIT-8403 and FIT-8404 meters and manipulate the power of the P-801 and P-802 pumps to adjust the inlet flow rate to the established range. If the values are higher or lower than the established values, the purity or recovery of the product will be reduced.

A clear example is the one that occurs in zone I where adsorption is carried out, since it is very important to control the feed flow rate, which is mainly linked to the volume of the pores of the column, sizing of the column. In the case of obtaining a very high value of feed, we would have insufficient adsorption and therefore a much lower recovery of p-xylene than desired, on the other hand, if we have a much lower flow rate, we would be wasting the sizing and elements of the column/process.

Switch time of the rotary valve

For the correct operation of the PAREX unit the most important element is the rotary valve developed by UOP, a very important element for its operation and that of the column is the Switch time, time in which the rotary valve switches the inputs and outputs in the column. Stipulating one full revolution as the cycle time.

This cycle time must be set and is controlled by level switches that send a signal when a full turn has been made (this is. 7 inputs or outputs have been present) on one of the

streams. Level switches LIT-8801 and LIT-8802, in case of a failure in this element it will be necessary to adjust the internal program of the valve.

Temperature control

The temperature control loop of the unit is simple as no exothermic or endothermic reaction takes place, so the temperature is controlled at the inlet flows by means of the level indicators before and after E-821 and E-822 by manipulating the steam inlet valve V-8202 and V-8203 until the desired value is obtained at the outlet of the flow.

Pressure control

The pressure is measured by the pressure gauges PIT-8503, PIT-8504, PIT-8505 and PIT-8506, respectively, and these values are transmitted to the pressure controller with their setpoint and transferred to the motor drives of the corresponding drive pumps for adjustment to the desired value.

5.3.3. Isomerization reactor

Pressure control

In the reaction zone, the pressure at the reactor inlet needs to be optimally regulated. In this case, the pressure is checked during the piping sections by means of the gauges, PIT-10201 and PIT-10207.

If this value deviates, the power supplied to the P-1051 motor is manipulated in order to increase the pressure at the pump discharge until the required pressure is reached.

Feed composition control

The reactor inlet must maintain a ratio between the hydrogen and the xylene mixture, so the flow rate supplied by FIT-10103 and the stream containing mostly hydrogen is measured with FIT-10101 and FIT-10102, manipulating the fresh hydrogen inlet with V-10003 to maintain the ratio between both streams.

Temperature control

The control of the reactor inlet temperature is performed by the fuel flow rate consumed in H-502, where heat is transferred between the inlet stream to the furnace and the reactor outlet, the detailed control was already described in the previous project

and the control loop of the corresponding equipment is shown. As this is a reaction without a significant temperature variation, there is no control in the equipment itself.

5.3.4. Gas-liquid separator

Pressure control

The separator head pressure gauges, PIT-10203 and PIT-10204, cause the V-10002 valve to be manipulated to keep the operating pressure constant, and the compressor motor to be manipulated to provide the required power, aided by the V-10003 inlet flow meter.

Level control

The separator level is measured by LIT-10401 and LIT-10401, in the event of a level deviation, the valve V-10003 is manipulated.

Temperature control

In the process of separating condensable and non-condensable, the most important part is the temperature control.

The temperature is measured by means of the TIT-10303 and TIT-10304 indicators, and the speed of the AE-1003 motor is manipulated. On the other hand, it is also possible to increase the residence time of the separator to be able to cool down a few degrees by closing V-10005.

In case of double action in V-10005, the level gauge prevails as the most restrictive element.

5.3.5. P&ID 13001

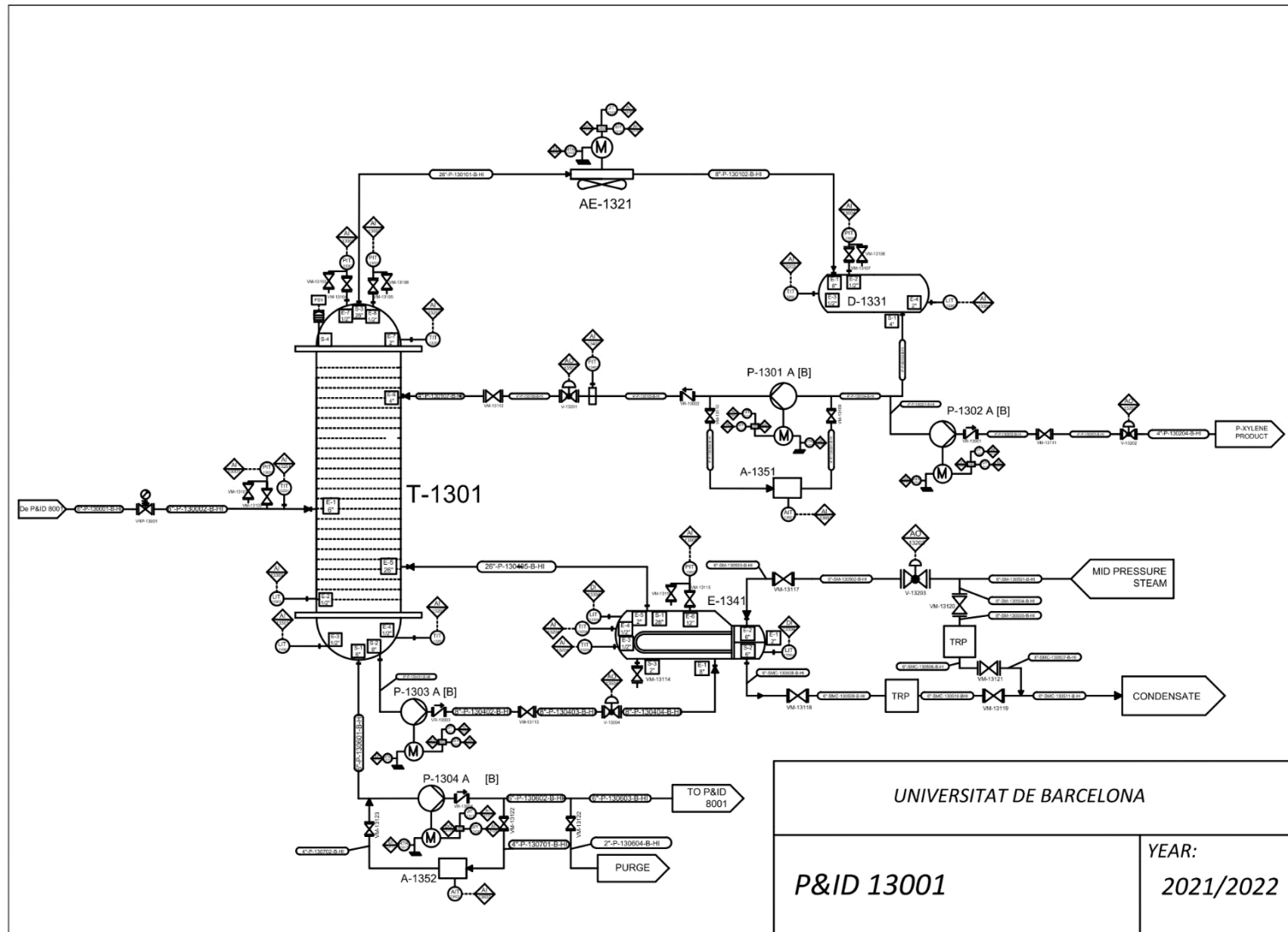


Figure 7. P&ID 13001.

5.3.5. P&ID 8001

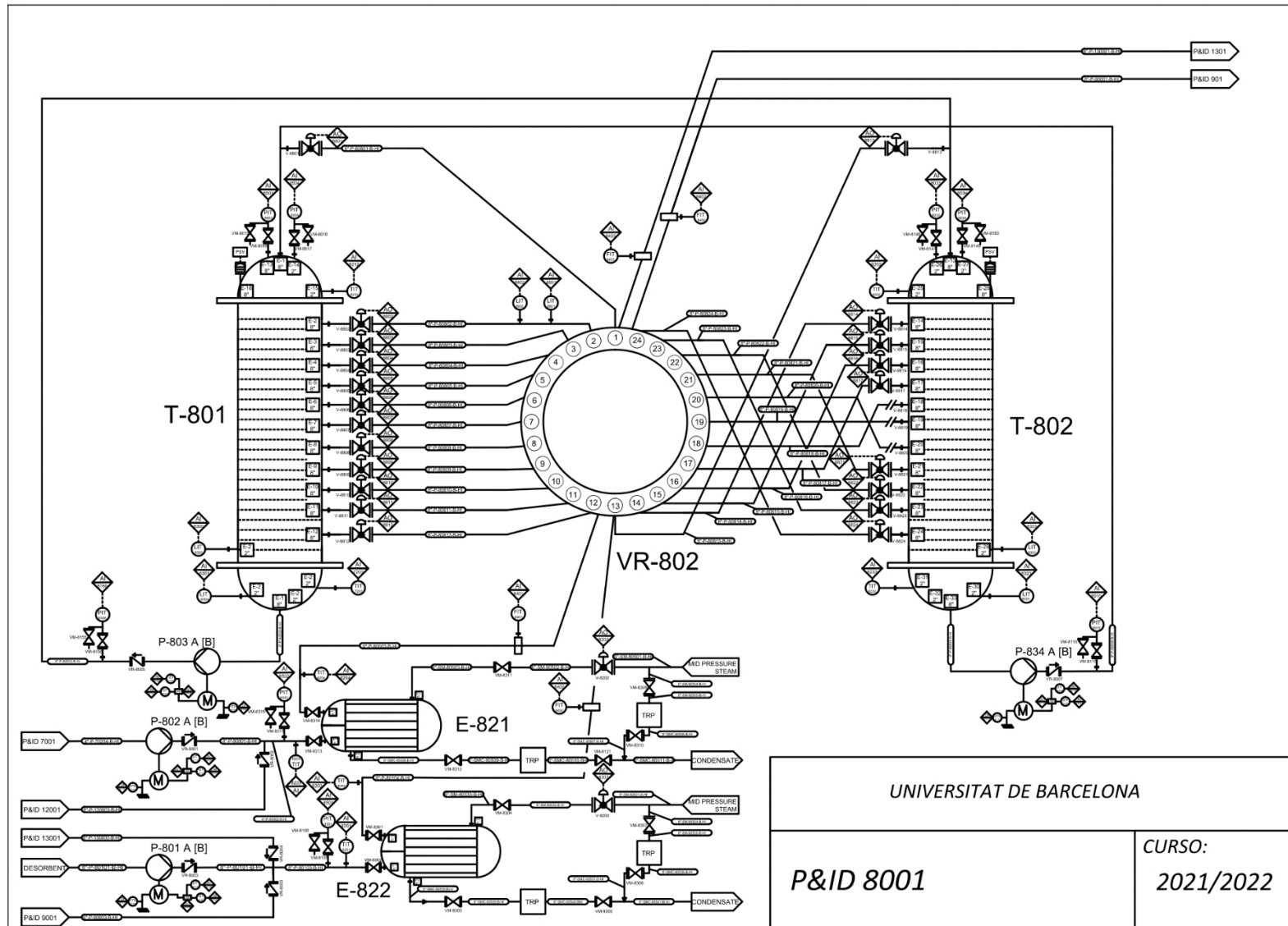


Figure 8. P&ID 8001.

5.3.5. P&ID 10001

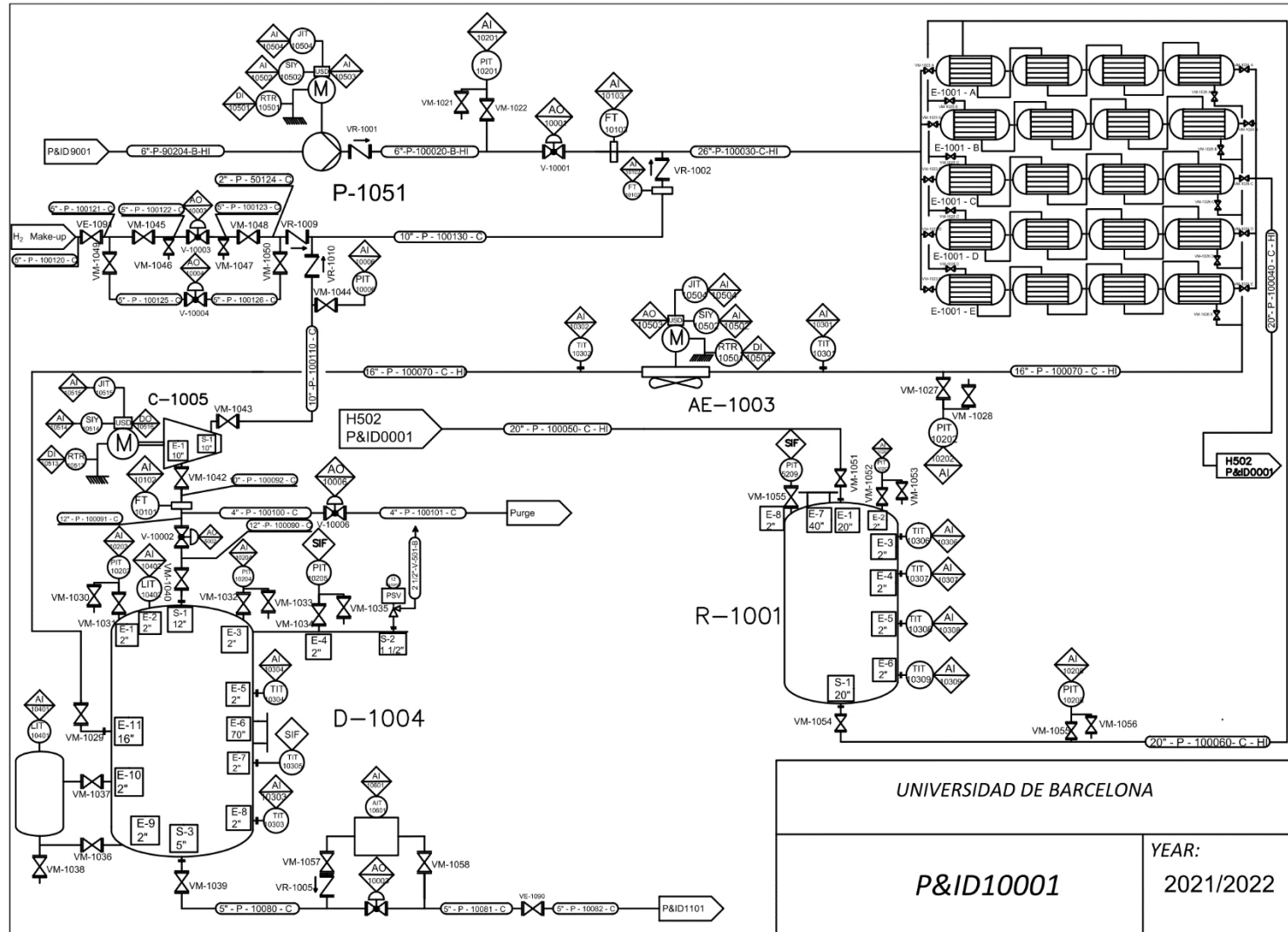


Figure 9. P&ID 10001.

5.4. Design of the equipment

5.4.1 Distillation column

Column T-601

The stream from reaction zone Z-500, where the disproportionation of the toluene is carried out to obtain benzene and p-xylene, the T-601 distillation column is designed to separate the benzene, the product, to the desired purity from the rest of the components that are recirculated to the T-301.

To estimate the equipment, the Short-Cut method is first applied in Aspen Plus, using the DSTWU column, obtaining a reflux value and a minimum number of trays, as well as knowing qualitatively where the feed is located. This calculation is done by marking a light compound, benzene, and a heavy compound, p-xylene. A benzene recovery of 99.998% per column head and a recovery per head of 0.001% of the heavy key were set. Subsequently, a rigorous simulation was carried out using the Rad. Frac unit, a 100 trays column, setting the purity and the benzene recovery per column head to corroborate the minimum flow rate and the flow rate necessary to obtain per head with respect to the feed, Table 1 shows the minimum stage and reflux values.

Table 1. Values for number of stages and minimum reflux.

Parameter	<i>Short-cut</i>	<i>Rad. Frac.</i>
Minimal stage	17	-
Stage	100	100
Minimal reflux	0.31	-
Operation reflux	0.35	3.52
Feed stage	60	50

As can be seen, there is a notable difference between the rigorous method and the short cut method because the short cut method is a method for mixtures that behave in an ideal way, so in this case the short cut method gives an erroneous result.

Therefore, for the value of the minimum reflux the rigorous method is used, a range of operating reflux is marked, this value is approximately around 1.2 - 1.5 of the minimum reflux. This value is described in the literature where they determine the optimum reflux between equipment cost, lower reflux plus number of trays, and service cost, higher reflux implies higher consumption.

The operation to find the number of trays and the operating feed stage is by means of a sensitivity analysis where the number of trays is reduced manually and for each change in the feed stage the reflux is calculated, once a value close to the desired operating reflux is obtained, the final configuration is obtained. Table 5 shows the final column design.

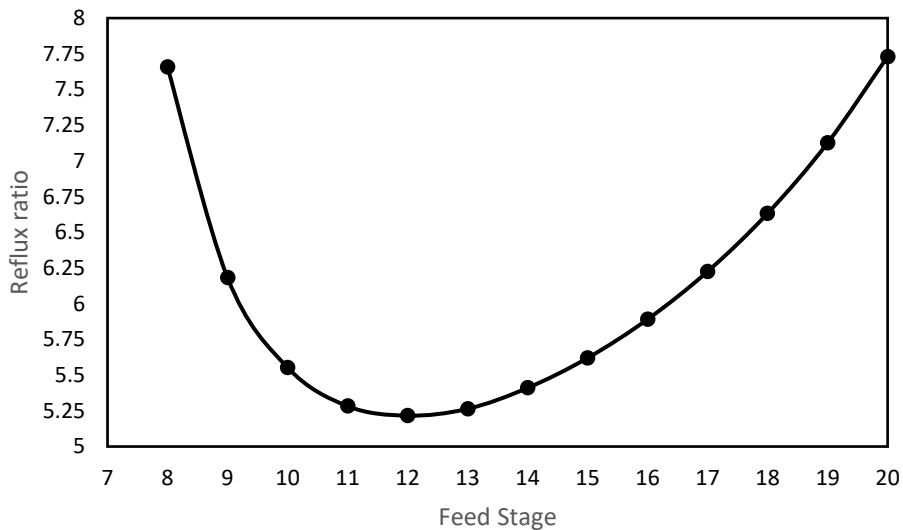


Figure 10. Sensitivity analysis column T-601.

Column T-701

After the toluene purification column, the bottom of the T-301 column is sent to the T-701 column in order to separate the heavier and more volatile compounds.

As in the previous case, the column is first estimated by the Short-Cut method using the DSTWU column, and the reflux value and minimum number of stages are obtained, in addition to knowing qualitatively where the feed is going to be located. For this separation, a column bottom recovery of 99.5 % of the compound was set.

A rigorous simulation was then carried out using the Rad. Frac unit, with a column of 100 trays and setting the recovery of o-xylene per column head at 99.8% and a recovery of 99.9% for methylbenzene in order to corroborate the minimum reflux.

Table 2. Values for number of stages and minimum reflux.

Parameter	<i>Short-cut</i>	<i>Rad. Frac.</i>
Minimal stage	33	-
Stage	100	100
Minimal reflux	1.58	-
Operation reflux	1.68	1.68
Feed stage	49	50

Once the minimum reflux value has been obtained by the Short Cut method and the rigorous method, an operating reflux range is set, this value is approximately around 1.2 - 1.5 of the minimum reflux.

As in the case before, the number of trays is modified, and a sensitivity analysis is carried out where the value of the reflux is observed with respect to the feeding stage in order to size the equipment.

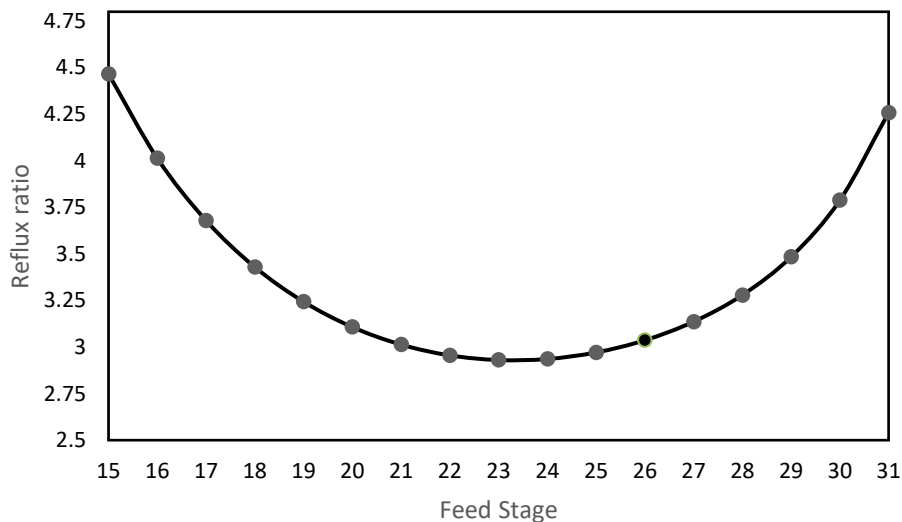


Figure 11. Sensitivity analysis of reflux with respect to feeding stage.

Column T-901 and T-1301

The two streams coming from the PAREX column, extract and refined, adsorption column where the separation of p-xylene from the other compounds is carried out, the T-901 and T-1301 distillation columns are designed and used to separate the desorbent from the mixture and recirculate it back to the adsorption column.

To estimate the column, as in the previous cases, the Short-Cut method is used in Aspen Plus. Table 3. shows the value obtained by setting a desorbent recovery of 0.001% of the desorbent per head and 99.9% of the light compound.

In the Rad. Frac unit, with 100 trays and setting the purity and the recovery per column bottom of the desorbent, the minimum flow rate and the flow rate through the bottom of the column with respect to the feed are obtained.

Table 3. Values for number of stages and minimum reflux.

Parameter	T-901		T-1301	
	Short-cut	Rad. Frac	Short-cut	Rad. Frac
Minimal stage	17	-	14	-
Stage	100	100	100	100
Minimal reflux	1.03	-	1.4	-
Operation reflux	1.06	1.19	1.45	1.62
Feed stage	49	50	57	50

Rigorous simulation is carried out until the operating reflux value is obtained, 1.2-1.5 minimum Reflux, in addition to the sensitivity analysis in order to define the feed stage as shown in Figure 12 and 13 respectively for each column. Table 5 shows the final column design.

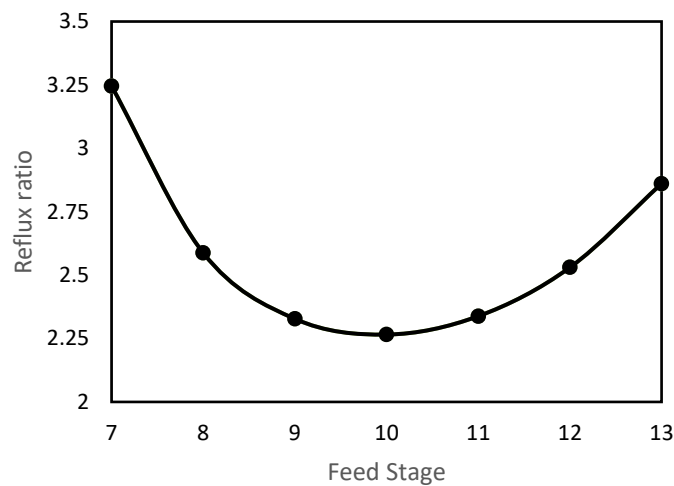


Figure 12. Sensitivity analysis of reflux with respect to feeding stage.

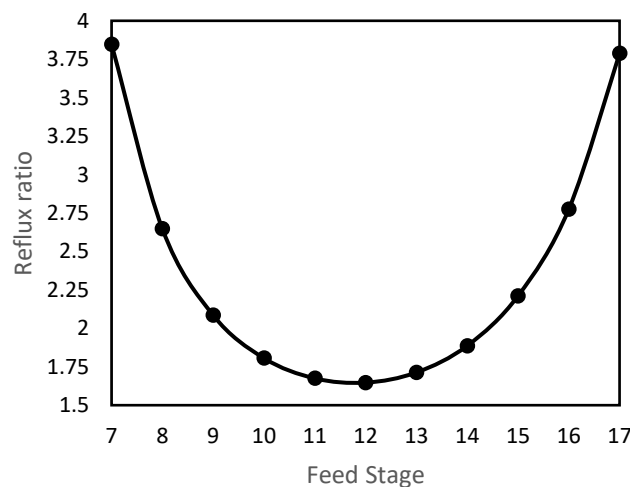


Figure 13. Sensitivity analysis of reflux with respect to feeding stage.

Column T-1201

The current coming from the Z-1000 reaction zone, the zone where the isomerization of xylene takes place, the T-1201 distillation column is designed in order to separate the benzene, produced in the reaction zone, to the desired purity from the rest of the components that are recirculated together with the T-401 head compounds to the adsorption column.

To estimate the equipment, the Short-Cut method is first applied in Aspen Plus, using the DSTWU column, obtaining a reflux value and a minimum number of stages, as well as knowing qualitatively where the feed is located. This calculation is done by marking a light compound, benzene, and a heavy compound, p-xylene. A benzene recovery of 99.998% per column head and a recovery per head of 0.001% of the heavy key were set. Subsequently, a rigorous simulation was carried out using the Rad. Frac unit, a 100-plate column, fixing the purity and the benzene recovery per column head to corroborate the minimum flow rate and the flow rate necessary to obtain the feed per head.

Table 4. Values for number of stages and minimum reflux.

Parameter	<i>Short-cut</i>	<i>Rad. Frac.</i>
Minimal stage	19	-
Stage	100	100
Minimal reflux	0.96	-
Operation reflux	1.01	1.61
Feed stage	35	50

As in the previous cases, the number of trays and the operating feed stage is found by a sensitivity analysis where the number of trays is reduced manually and for each change of the feed stage the reflux is calculated, once a value close to the desired operating reflux is obtained, the final configuration is obtained. Table 5 shows the final column design.

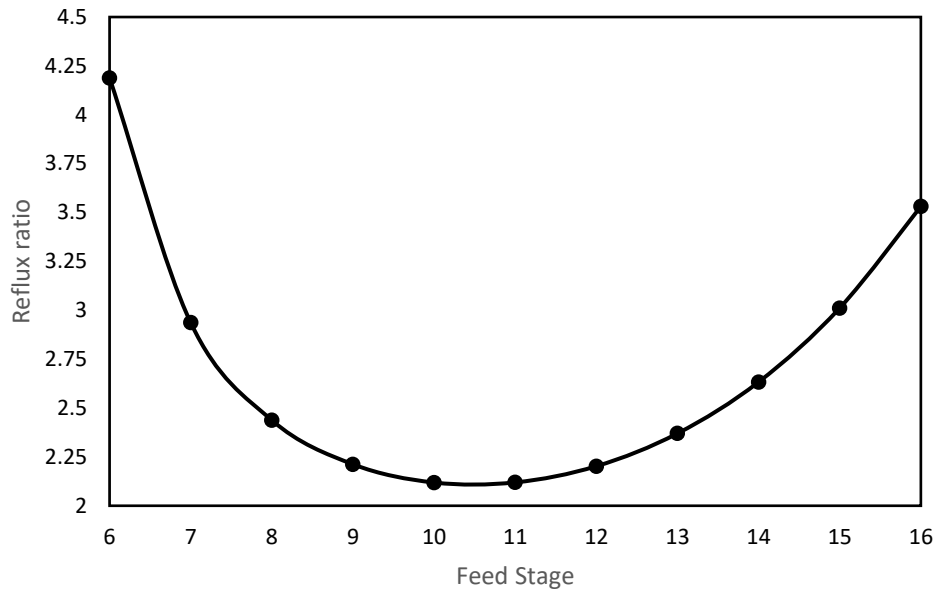


Figure 14. Sensitivity analysis of reflux with respect to feeding stage.

Table 5. Column characteristics.

Parameter	units	T-401	T-701	T-1301	T-901	T-1201
Column head pressure	bar(a)	1	1	1	1	1
Column bottom pressure	bar(a)	1.33	1.37	1.15	1.15	1.26
Column head temperature	°C	83	139	138	138	79.8
Bottom of column temperature	°C	125	176	189	189	145
Theoretical number of plates	-	34	42	22	23	29
Feed stage	-	12	23	10	12	10
Reflux ratio	-	5.22	2.89	2.27	1.65	2.35
Pressure drop per tray**	bar(a)	7.00·10 ⁻⁰³				

*In the columns, the total stages include total condenser and the Kettle reboiler.

**The pressure drop per plate is established by obtaining a bibliographical value that for columns operating at atmospheric pressure the value is 0.007 bar(a).¹⁴

Column Internal

Once the number of trays, reflux and feed stage have been characterized, the internal design of the column is carried out using ASPEN PLUS.

In all cases, the design provided divides the column in two, from the first stage to the feed stage and from the feed stage to the last stage. Different diameter values can be given, at industrial level this differentiation is applied if there is at least 0.2 meters between the two zones. If this value is lower, the value of the upper diameter is selected, oversizing the column.

There may not be a difference in diameter, but it is possible that there may be two different configurations of trays and internal dimensions, as it is necessary to analyze how each tray works for the correct operation of the column, as shown in Figure 15.

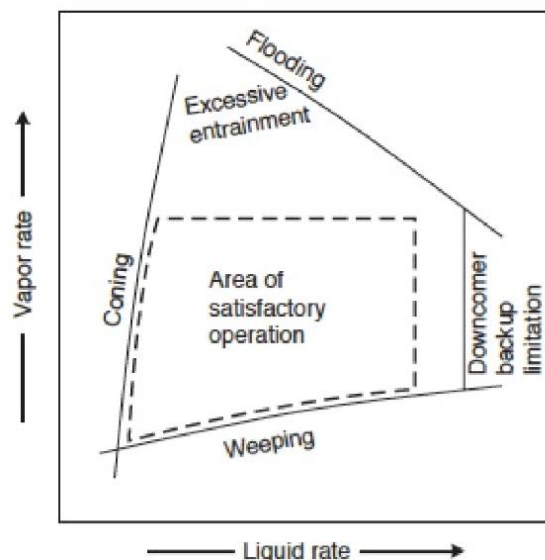


Figure 15. Operating conditions of the column trays.

In case a tray does not work in the correct operating range, the following problems may occur:

Coning: liquid rate too low. The vapor moves the liquid away from the slots and flows through it as a continuous stream. No/no vapor/liquid mixing.

Dumping: vapor rate too low. Some slots dump liquid and do not pass vapor. Vapor accumulates and eventually passes through as a pulse.

Weeping: combination of pulsating vapor flow and pouring.

Flooding: vapor rate too high. This creates a retention of liquid on the plate. It creates an increase in the pressure drop of the column.

Carryover: high vapor flow carries liquid back up the column to the previous tray. The upper limit is 0.1. Below this value, the effect of entrainment on efficiency is small.

Foaming: the liquid expands due to the passage of vapor. Although a large vapor-liquid interfacial area is created, foaming can cause strong liquid retention in a tray. The vapor rate should be lower

Therefore, it is necessary to check each tray of the column and modify certain parameters to work in the described area. The characterization and resolution procedure of the internals is shown in Appendix 2.

Table 6. Internal dimensions of the distillation columns.

	T-601		T-401		T-901		T-1201		T-1301	
	Section		Section		Section		Section		Section	
	1	2	1	2	1	2	1	2	1	2
Diameter (m)	2.86	3.33	3.6	3.6	4.4	4.73	1.06	2.42	2.81	3.02
Number of passes	1	1	1	1	1	1	1	1	1	1
Total area (m ²)	6.42	8.71	8.16	8.16	15.2	17.6	0.881	4.61	6.2	7.22
Active area (m ²)	5.13	6.97	10.2	10.2	12.2	14.1	0.705	3.69	4.95	5.78
Tray spacing (mm)	610	715	610	722	610	856	610	721	610	735
Jet Flood	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8
Weir height (mm)	50.8	59.6	50.8	60.2	50.8	71.3	50.8	60.1	50.8	61.3
Downcomer clearance (mm)	38.1	54	38.1	47.5	38.1	69.1	38.1	53.2	38.1	48.6
Downcomer width top (cm)	44.7	52.1	56.9	55.1	68.9	74.1	16.6	37.9	43.9	47.5

5.4.2 Adsorption Column (T-801 and T-802)

The design of the adsorption column, which uses the technology described above, follows the literature, which describes the adsorption column on an industrial scale.¹⁰ Other bibliographic sources simplify the column design and reduce the number of beds, making their microscopic resolution simpler and unrealistic on an industrial scale.¹⁵

In order to characterize the adsorption column, the first step is the resolution of the balance of matter of the unit, knowing that on an industrial scale a recovery of p-xylene of 92.5 % in mole fraction is obtained in addition to obtaining a purity with respect to the other compounds, excluding the desorbent, of 99.65 % in mole fraction. It must be considered that the distribution of the rest of the species in the extract is proportional to the inlet flow rate. The recovery and purity values are conservative as they may fluctuate depending on the type of feed in the column. The equations describing the resolution of the mass balance can be found in Appendix 3.

It must be considered that at industrial level, 24 beds are operated in two chambers of 12 beds, both columns connected to each other. The column does not only operate with 2 inlet lines (desorbent and feed) and 2 outlet lines (extract and refined), but also has a washing inlet (recirculated desorbent) and 2 outlets, washing and secondary washing (desorbent and feed), which have the function of eliminating possible cross-contamination of the extract. Therefore, the column is not divided into 4 sections, but has a total of 7: I, IIA, II, IIB, III, IIIA and IV, due to the entry and exit points of the washes. The movement of the profile within the column that describes the SMB model is industrially carried out by means of the rotary valve that periodically and synchronously switches the seven inlets/outlets. The switching time is a parameter to be calculated to characterize the equipment (diameter and height of the beds).

For this purpose, once the material balance of the unit has been calculated, the equations described in Appendix 3 for the characterization of the internal parameters and flow rates are solved.

Once the values have been characterized, it is possible to size the column, the equipment characteristics are shown in Table 7.

As defined in the technology review, the catalyst used is hydrated Y or X-type faujasite where the compound that has the potential to make physisorption is p-xylene.

The internal flow rates of the column are shown in Table 8.

Table 7. Unit characteristics.

Adsorbent Chamber				Dead Volumes*				
Number of beds/adsorbent chamber	12	Bed head	L_{BH} , m	0.22				
Diameter (m)	4.41		D_{BH} , m	4.27				
Total length (m)	13.9	Bed lines	L_{line} , m	17.8				
Chamber length (m)	1.15		D_{line} , m	0.127				
Cycle time (h)	0.68	Circulation lines	L_{circ} , m	25				
Switch time (s)	101		D_{circ} , m	0.203				
Rotary valve (configuration)				Unit's selective and nonselective volumes				
I	IIA	II	IIB	III	IIIA	IV	$V_{selective}$, m ³	69.2
7	2	6	1	4	1	3	$V_{non-selective}$, m ³	208
Adsorbent		m^{total} , kg		298714		ρ_{bed} , kg/m ³	896	
		ϵ_{bulk}		0.390		$\rho_{particle}$, kg/m ³	1480	
		$\epsilon_{particle}$		0.360		r_{porus} , mm	0.3	

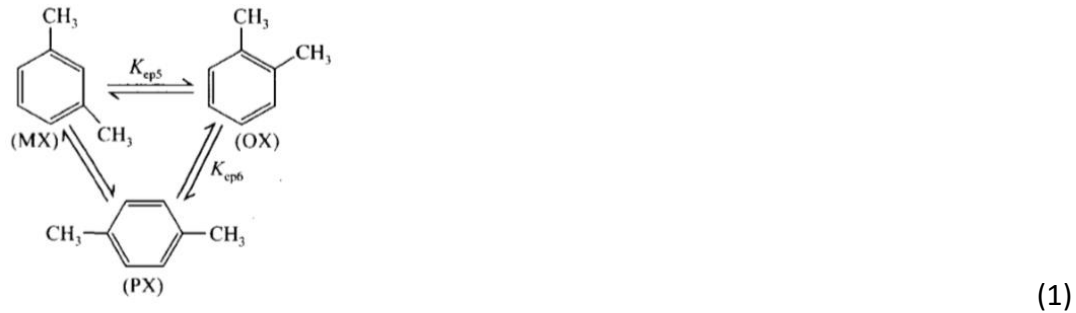
*These values are obtained bibliographically.¹⁰

Table 8. Internal column flow rates.

Variable		Value	Unit
Flow rate zone II	QII	244.97	m ³ /h
Flow rate Zone III	QIII	275.85	m ³ /h
Flow Zone IV	QIV	196.31	m ³ /h
Flow Zone IIA	QIIA	255.58	m ³ /h
Flow rate Zone I	QI	316.68	m ³ /h
Flow Zone IIB	QIIB	236.80	m ³ /h
Flow Rate Zone IIIA	QIIIA	286.47	m ³ /h
Flow rate Desorbent	QD	90.16	m ³ /h
Extract Flow Rate	QE	39.05	m ³ /h
Refining Flow Rate	QR	120.37	m ³ /h

5.4.3 Isomerization reactor R-1001

The main reaction of the isomerization reactor is the equilibrium of the three isomers, para-xylene, meta-xylene and ortho-xylene, by modifying the position of the radical as shown in Equation 1. ¹⁶



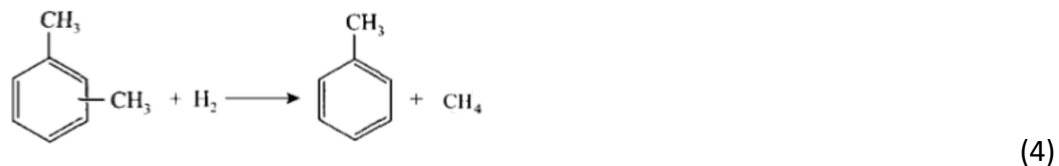
In addition to the dealkylation reaction of ethylbenzene to produce benzene and ethane as shown in Equation 2.



Due to the other compounds present in the isomerization reactor the following side reactions occur which depend on the operating conditions of the reactor such as the trans alkylation of xylene to toluene and trimethylbenzene as shown in Equation 3.



Or the hydrogenolysis reaction where xylene reacts with hydrogen to form toluene and methane as shown in Equation 4.



Catalyst

The catalyst used is zeolite ZSM-5, this type of zeolite is a hydrated aluminosilicate with a general formula shown in Equation 5. ¹⁷



The zeolite structure is made up of tetrahedrons generating a first primary structure which is joined with other tetrahedrons generating the unit called pentasil. This pentasil joins together generating a chain that subsequently generates a three-dimensional network as shown in Figure 16.¹⁸

This type of catalyst is already present in the process, specifically in the toluene disproportionation reactor, in that case it was modified with silicate to reduce the pore size.

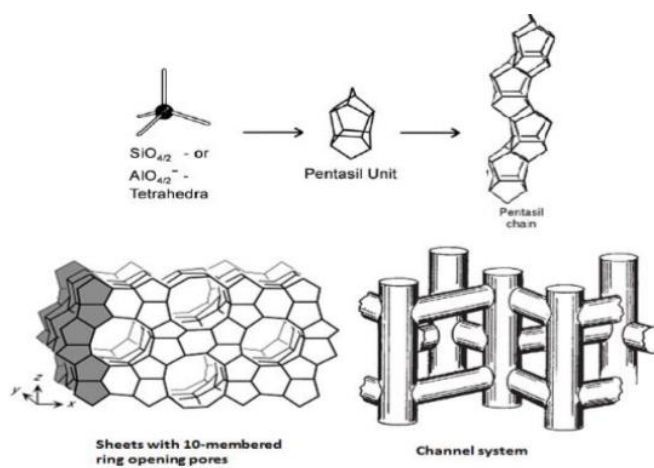


Figure 16. Structure of zeolite ZSM-5.

(Image extracted from ref. 18)

This type of catalyst favors the exclusion of certain side reactions due to its three selectivity.

Reactive selectivity: The catalyst excludes certain molecules due to their size, allowing smaller molecules to flow through the pores.

Product selectivity: The catalyst does not allow the product generated to diffuse inside it, in the case of a large size, remaining, retaining it inside.

Transition state selectivity: It does not generate other compounds because they are larger than the pore size.

Operational condition^{16, 19, 20}

For the correct operation of the isomerization process and to obtain a high selectivity to the desired compound, the principal variables are campaign lifetime, temperature,

hydrogen partial pressure, space velocity (WHSV) and hydrogen/hydrocarbon molar ratio.

The campaign lifetime is coupled with the operation of other process units such as the toluene disproportionation reactor.

As the temperature increases, the isomerization approaches equilibrium, while the cracking reactions increase their yield. To determine the operating temperature, it is necessary to know the deactivation temperature of the catalyst, which is higher than 420 °C. Thus, the normal operating temperature range in the C8A isomerization system is in the range of 345 to 420 °C.

Hydrogen pressure affects the reaction rate as these are concentration-dependent, although higher pressure favors ethylbenzene saturation reactions and makes dealkylation less favorable. Typically, the hydrogen partial pressure range varies between 5 and 10 bar.

The space velocity (WHSV) is described by the unit as it does not change, only by the amount of input feed.

The hydrogen/hydrocarbon molar ratio affects in several ways, increasing the molar ratio increases the lifetime of the catalyst because it favors the precursors that generate the Coke, while it is possible that it favors other side reactions. The typical operating value of the H₂/HC ratio varies between 2 and 5.

Equipment characterization

Table 9 presents the main characteristics of the reactor and specifies the catalyst used, specifically from the company Clariant.²¹

Table 9. Characteristics of the reactor.

Variable	value
Catalyst	ZSM-5; ISOXYL MPH ²¹
Operational condition	
Reactor type	Fixed bed
Temperature (°C)	420
Pressure (bar)	10
H ₂ /HC (mol)	2.5
WHSV	1.8
conversion EB(%)	80
Equilibrium (%molar)	
p-xylene	26

o-xylene	56
m-xylene	18
Loss production xylene (%)	1.2
Sizing	
Catalyst (kg)	45000
Diameter (m)	2.55
Height (m)	8.55
Bed density (kg/m ³)	915

5.4.4 Heat exchanger E-1001

The simulation and design of the E-1001 heat exchanger that preheats the input stream to the isomerization reactor with the output stream of the reactor has been carried out. The first step is to know the energy that needs to be transferred, this being a total of 239523 kW, defining that the energy transfer between the two fluids cannot exceed 40 degrees, to ensure correct operation and that in this case it makes no difference whether the fluid circulates on the shell side or the tube side as they have the same behavior, the design is carried out with Aspen Exchanger. Table 10 shows the main characteristics of the E-1001 heat exchanger:

Table 10. Design data of E-1001.

Variable	Value
Heat Exchanged (kW)	23953
Transfer rate (W/(m ² K))	300
Surface/unit (m ²)	3209.2
Configuration:	BEM: 5 parallel 4 serie
Surface/Shell (m ²)	160.5
Size of shell (mm)	675 - 4950

Figure 17 shows the temperature profile within the 4 heat exchangers. It can be seen that at no point is there a crossover of temperatures in the correct operation of the set of exchangers. Appendix 4 shows the specification sheet of the Heat Exchanger.

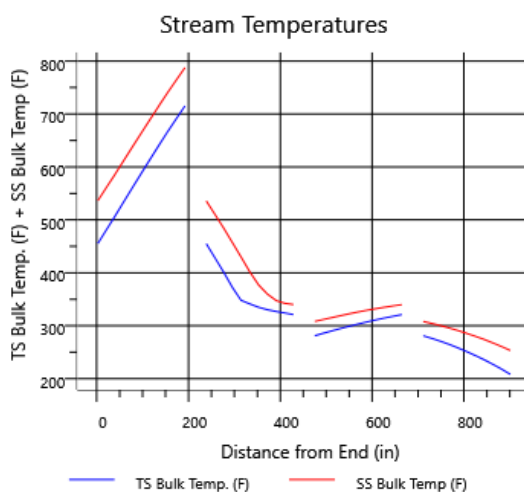


Figure 17. Temperature profile of the heat exchanger assembly.

5.4.4 Furnace H-502

The H-502 furnace has been resized, as it had the capacity to heat the fluid that entered only the toluene disproportionation reactor, with a contribution to the process of 2000 kW. The new process furnace, H-502, must have the capacity to supply not only the needs of the process but also to heat the fluid with 25 % more excess, specifically 6000 kW.

As in the first furnace design, energy is provided by the combustion of natural gas because it is the equipment with the lowest emissions of gram of CO₂ per useful kWh generated of the various heat sources.

Specifically, natural gas produces around 25-30 % less than oil derivatives and even 40-50 % less than coal-fired boilers. Another important fact is that natural gas does not produce Sulphur compounds.²²

The composition of the natural gas for which the calculations have been made is shown in Table 11 together with the enthalpy of combustion of the compounds.

Table 11. Composition of natural gas ²³.

Compound	Composition (%Volume)	Enthalpy of combustion (kJ/mol)
Methane	91.5	-802
Ethane	7.1	-1321
Propane	0.7	-2044
Butane	0.1	-2649
Nitrogen	0.6	-

In order to estimate the necessary flow rate of the system, it is assumed that the reaction is complete, and that the nitrogen does not react to generate NO_x.

The combustion reactions are shown below.



Behaving as an ideal gas, the volumetric composition is the same as the molar composition, and therefore the enthalpy of combustion of one mole of natural gas is estimated by Equation 10. Where it is obtained that the heat of combustion of natural gas has a value of -845 kJ/mol.²³

$$\Delta H_{combustion} = \sum \Delta H_{combustion,i} \cdot x_i \quad (10)$$

After calculating the enthalpy of combustion of natural gas, the required flow rate is calculated, estimating the furnace efficiency to be 84%, that show in the Equation 11.²³

$$W_{natural\ gas} = \frac{Q}{\Delta H_{combustion} \cdot 0.84} \quad (11)$$

The flow rate obtained is 550 kg/h of natural gas.

The furnace has two parts, the part where the fluid is heated by radiation, located in the lower part of the furnace, where the tubes are mounted vertically in order to improve heat transfer, and in the upper part, due to the fact that the exchange is carried out by convection, the tubes are horizontal; Figure 18 shows a diagram of the equipment.²⁴

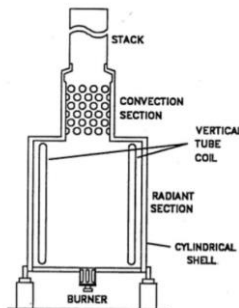


Figure 18. Representative schematic of H-502.

(Image extracted from ref. 24)

If we analyze the part of the natural gas, it enters a burner, which is located at the bottom, and generates the fumes that go up to the chimney, in the chamber there is always a percentage of excess oxygen of 5 %, in order to control the correct regulation. The oven works by natural draught and has a valve in the chimney to regulate the air flow.

The P&ID of this unit was carried out during the development of the reference project, modifying the inlet lines to the unit. P&ID shown in Appendix 1.

5.4.5 Separator D-1004

The D-1004 separator has the function of separating the condensable from the incondensable present in the reactor stream to recirculate the hydrogen into the reactor, so that the imposition of the operating conditions has the function of reducing the amount of product going into the incondensable stream.

The temperature has a lower limit of 32 °C, as the aerorefrigerant, A-1003, is used for the cooling of the current, and this allows a maximum of 32 °C, the use of aerorefrigerant is due to the lack of cooling water in the existing plant.

On the other hand, there is no limit to the range of pressure that can be varied, but no equipment will be incorporated to increase the current pressure.

Therefore, both operating conditions are plotted within the range to corroborate the optimum operating conditions, the values are shown in Figure 19.

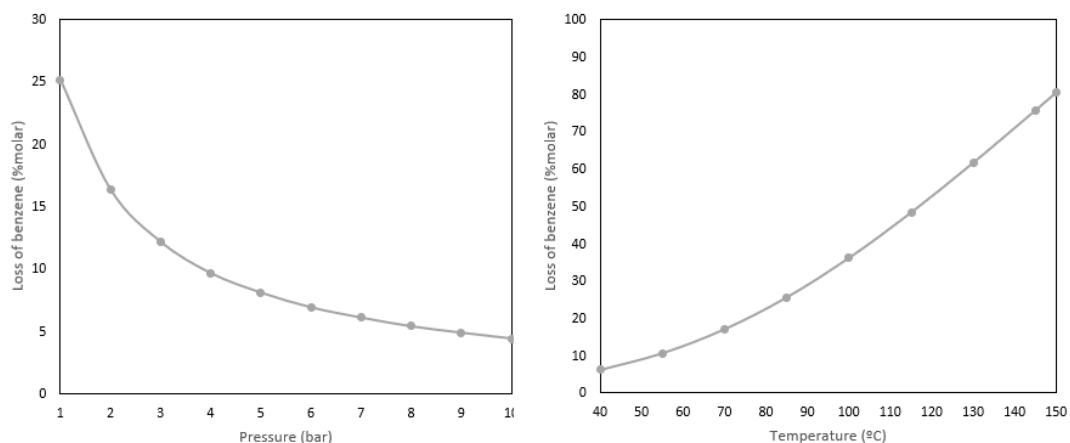


Figure 19. Benzene loss as a function of operating conditions.

The best operating conditions are to keep the temperature as low as possible 40 °C a higher pressure.

Sizing²⁵

Once the operating conditions of the equipment have been defined, the sizing of the equipment is carried out, for which it is first necessary to know the minimum diameter to efficiently separate the gas from the liquid, this is done by means of Equation 12.

$$D_{min.} = \sqrt{\frac{4 \cdot V'}{\pi \cdot u_s}} \quad (12.)$$

Where u_s is directly related to the design and to the variable u_t , which is defined as the liquid deposition rate calculated in Equation 13.

$$u_t = 0.07 \cdot [(\rho_l - \rho_v) / (\rho_v)]^2 \quad (13)$$

The value of u_s is equal to the Equation 5.13 value if this separator is designed with a demister, an element used to separate the droplets, or 0.15 the Equation value 13 if it is designed without one.

According to the bibliography, the height of the equipment is a function of the diameter as shown in Figure 19, and the liquid level must contain at least 10 minutes residence time in order to ensure proper control.

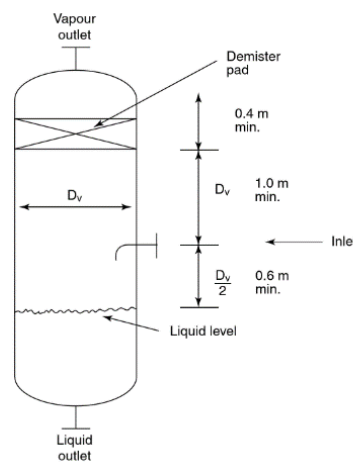


Figure 19 Sizing of the equipment.

(Image extracted from ref. 25)

Table 12 below shows the minimum values for height and diameter.

Table 12. Minimum dimensioning values.

Variable	D. without demister	Total height without demister	D with demister (m)	Total height with demister
Valor	1.25	5.58	3.23	2.54

An optimization of the equipment dimensioning is carried out to reduce the external surface of the cylinder, as this reduces the cost of the equipment.

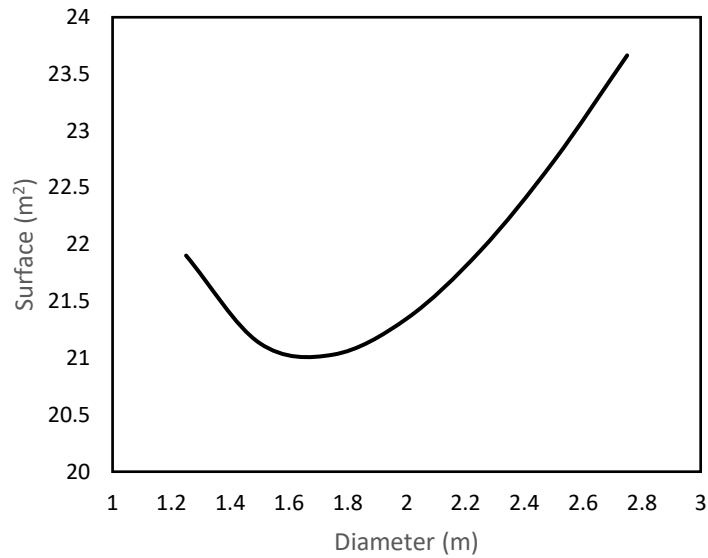


Figure 20. Analysis to reduce the external surface of the cylinder.

Table 13. Final sizing of the equipment.

Variable	Diameter (m)	Height (m)	Design pressure (bar)	Design temperature (°C)	Thickness (mm)
Value	1.67	4.03	15	410	20

The thickness of the equipment has been calculated using the following equations, both for the 2:1 ellipsoidal head, Equation 14. and the cylindrical body, Equation 15.²⁶

$$t_{head} = \frac{Pd \cdot D}{(2 \cdot S \cdot E - 0.2 \cdot Pd)} + CA \quad (14)$$

$$t_{cylindrical \ body} = \frac{Pd \cdot r}{(S \cdot E - 0.6 \cdot Pd)} + CA \quad (15)$$

Corrosion value with 3 mm

5.4.6 Piping design

In this section, the calculation of the diameter necessary to comply with the typical velocities of non-viscous fluids in pipes is carried out, which varies from 1-3 m/s for liquids and from 10-30 m/s for gases.

By means of the value of the volumetric flow, Equation 16 is used to determine the required flow area and, knowing that it is a circular area, to know the diameter of the pipe.

$$A = \frac{V'}{v} = \pi \cdot \frac{D^2}{4} \quad (16)$$

Considering that at industrial level there are pipe diameter standards, the value of the calculated diameter is considered to choose a pipe with a close diameter and after selection, the velocity of the fluid in the pipe is recalculated to corroborate that it is within the desired range.

After calculating the diameter of the pipe, the minimum thickness necessary to resist the pressure of the interior is calculated.

In this case, Equation 17 is used to calculate the thickness, and the pipe model is chosen in conjunction with the desired diameter.²⁶

$$t_{pipe} = \frac{Pd \cdot D}{2 \cdot (S \cdot E + P \cdot 0.4)} + C \quad (17)$$

The value of 0.85 is used for electric arc welding, as prevention and over design and the value of 3mm is used as allowable corrosion, to increase the lifetime of the pipes.

The pipe pressure is determined by the highest-pressure value along the pipe. This includes the pressure drop and the pressure applied by the liquid.

After getting the specific model, the fluid velocity is recalculated to check if it complies with both the typical velocity and the minimum thickness.

Thermal Insulation

In order to work at high temperatures, it is necessary to insulate the pipes both for the energy efficiency of the plant, thus reducing the consumption of natural gas, and for the safety of the workers, as they cannot be in contact with surfaces above 50 °C.

Following the standard, the insulation from the company Isover Saint Gobain is used, specifically the ULTIMATE Wool Blanket model.²⁷

The thermal conductivity of the model varies as a function of temperature by the correlation as shown in the Equation 18.²⁷

$$k_{ins.} = 4E^{-7} \cdot T^2 + 6.77E^{-5} \cdot T + 3.26E^{-2} \quad (18)$$

And the conductivity of the pipe material also varies as a function of temperature by the correlation as shown in the Equation 19. ²⁸

$$k_{pipe} = -0.033 \cdot T + 55 \quad (19)$$

Figure 21 shows the scheme of heat transfer inside a cylindrical element to the outside. ²⁹

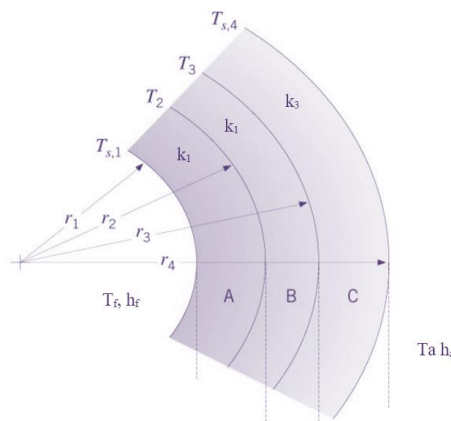


Figure 21. Scheme of heat transfer inside a cylindrical element.

(Image extracted from ref. 29)

Making the similarity with figure 21, the layer A indicates the thickness of the pipe, B the thickness of the insulation and C the coating of the pipe.

To determine the thickness of the insulation, Equation 20 is used, which calculates the temperature in the final coating through heat transfer. ²⁹

$$T_{s,4} = \frac{(T_f - T_a)}{r_4 \cdot h_a \cdot (R_1 + R_2 + R_3 + R_4 + R_5)} + T_a \quad (20)$$

The terms Ri describes the resistance to heat transfer, which is defined in two different forms, depending if it is convection which uses Equation 21 or conduction which uses Equation 22.

$$R_{conv} = \frac{1}{r_i \cdot h_i} \quad (21)$$

$$R_{cond} = \frac{\ln(r_o/r_i)}{k_1} \quad (22)$$

In this case and as described in the Figure 21, the value of R₁ is negligible since it is considered that the temperature inside the pipe is equal and there are no temperature gradients, this can be assured since it has always worked in turbulent fluid.

Substituting correctly the convection and conduction resistance in the general Equation, we obtain the Equation 23 which describes the heat transfer for this case and can be

used for the calculation of the insulation thickness by means of the unknown of the external radius, the thickness of the final cladding is 1 millimeter.

$$T_{s,4} = \frac{(T_f - T_a)}{(r_3 + 0.001) \cdot h_a \cdot \left(\frac{\ln(r_2/r_1)}{k_1} + \frac{\ln(r_3/r_2)}{k_2} + \frac{\ln((r_3 + 0.001)/r_3)}{k_3} + \frac{1}{(r_3 + 0.001) \cdot h_a} \right)} + T_a \quad (23)$$

The resolution is done with the Solver tool and as mentioned the surface temperature is below 50 °C.

On the other hand, the pressure loss in the pipes was determined, taking into account one meter of pipe and knowing the roughness of the pipe (ϵ), with a value of 4.5 millimeters.

The correlations of Swanee and Jain (1976), Haaland (1983) and the Darcy factor correlation were used. The calculations are shown in Appendix 5.

Table 14 shows a part of the pipeline list together with the P&ID and PFD numbering, the complete list is shown in Appendix 6.

Table 14. Part of the pipeline list.

Nº PFD	Nº P&ID	Diameter (inch)	Velocity (m/s)	Model	Pressure drop (cm /m pipe)		Insulate thiknes (mm)
					Haaland		
16	12"-P70002-B-HI	12.00	3.75	Std 40	2.86		14.9
17	4"-P70204-B-HI	4.00	1.58	Std 40	5.99		12.2
19	2"-P70602-B-HI	2.00	1.65	Std 40	14.52		17.2
42	4"-P80001-B-HI	4.00	1.58	Std 40	6.00		12.3
43	6"-P80002-B-HI	6.00	2.07	Std 40	5.54		13.3
44	6"-P80003-B-HI	6.00	2.16	Std 40	5.77		19.0
45	8"-P80101-B-HI	8.00	0.74	Std 40	0.40		19.9
49	6"-P130001-B-HI	6.00	0.42	Std 40	0.14		19.9
50	8"-P130002-B-HI	18.00	3.12	Std 40	3.21		18.3
51	4"-P130204-B-HI	4.00	1.20	Std 40	3.72		12.2
52/53	6"-P130602-B-HI	6.00	1.66	Std 40	4.79		21.9
56	8"-P90001-B-HI	8.00	1.99	Std 40	3.63		19.4

5.4.7 Pump selection (P-1051)

The process pump P-1051 has been characterized in order to show the pump selection criteria.

The P-1051 pump is used to increase the pressure of the stream to the pressure of the isomerization reactor.

The first step in pump selection is to obtain the total delivery head of the pump, which is obtained by Bernoulli's equation isolating the pump head as show in the Equation 24.³⁰

$$h_b = \frac{P_2}{\rho_2 \cdot g} - \frac{P_1}{\rho_1 \cdot g} + \frac{v_2^2}{2 \cdot g} - \frac{v_1^2}{2 \cdot g} + z_2 - z_1 + h_f \quad (24)$$

The value of hf described as the major and minor losses in the pipeline, explained in Appendix 5.

After obtaining the total pressure head of the pump, the discharge pressure of the pump can be found by means of Equation 25.

$$Pdch = h_b \cdot \rho_2 \cdot g \quad (25)$$

The available NPSH is then calculated, which is then checked when selecting the pumps to ensure that the value is greater than the NPSH required by the manufacturer to avoid cavitation.

Table 15 shows the value of the flow and the values obtained for the selection of the pump.

Table 15. Data for pump selection.

Variable	Value
Pressure (Pa _g)	0.1
Saturation pressure (Pa _g)	8550
Density (kg/m ³)	762
Head of bomb (m)	209
Flow (m ³ /h)	105
NPSH disp.	4.39

Given the values obtained for pump head and flow rate, a search is carried out in the standard manufacturers, where it can be seen that Grundfos does not have this type of pump, choosing the manufacturer Sundyne as it has high-pressured pumps that meet the requirement.

Looking in the catalogue, the Marelli-BB3,³¹ with model 3x4x9 as shown in Figure 22 is selected. The required flow rate is oversized due to the possibility of some fluctuations.

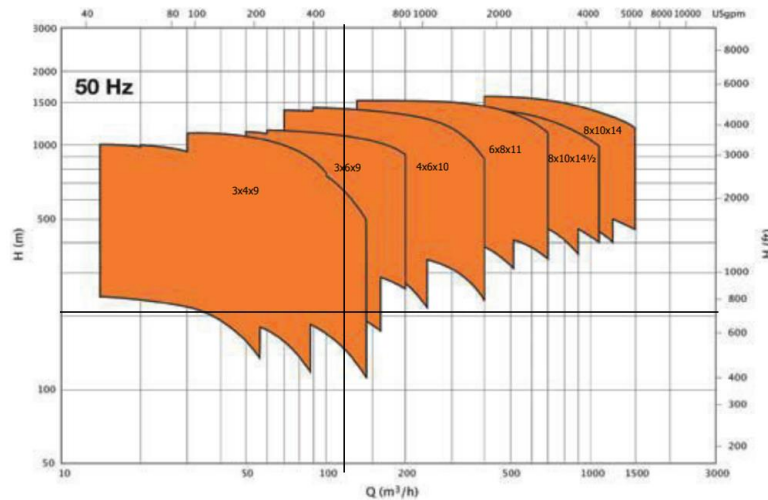


Figure 22. Selection model of the pump.

(Image extracted from ref. 31)

5.4.7 Safety relief valve (PSV)

The safety valve is a pressure relief system where its main function is to protect the equipment from a pressure inside the equipment that is higher than the design pressure, as this would be considered a rupture of the equipment.

The standard of the reference project is that as a minimum all equipment must withstand vacuum, the presence of air in the process is a handicap, and a minimum design pressure of 3.5 bar

The selection of a PSV over other types as a rupture disc is due to the fact that the process fluids do not polymerize and do not block the outlet in the PSV.

The design variable for the pressure relief valve is the gas flow rate at normal conditions that needs to be relieved from the system, to quantify this flow rate it is necessary to know the reasons for the pressure increase. The pressure increase in different systems can be caused by different options and needs to be analyzed individually.

One reason for pressure rises independent of the equipment of which the PSV is being sized, is external fire, the calculation for the flow rate due to external fire is shown in Appendix 7.³²

Once the flow rates are obtained, the biggest flow rate to be released is chosen and Equation 26 is used to obtain the valve orifice ³³. The method of calculation may vary from manufacturer to manufacturer.

$$A = \left[\frac{W}{387.2 \cdot C \cdot P \cdot K} \right] \sqrt{\frac{ZT}{M}} \quad (26)$$

Characterization of safety relief valve on T-1301

In the case of the distillation column T-1301, 3 possible scenarios have been taken into account, external fire, rupture of the kettle reboiler tube entering steam at 41 bar(g) and failure of the air coolant A-1331. Table 16 shows the value of the three situations.

Table 16. Discharge flow rate according to scenarios.

Variable	Unit	Value
Tare pressure	bar g	3.50
Operating temperature	°C	96.1
W fire	kg/h	3.65E+04
W air coolant failure	kg/h	8.73E+04
W tube burst	kg/h	45.02

Knowing the biggest discharge flow rate, by means of Equation 5.26, the orifice area is characterized and the model is chosen, the result obtained is shown in Table 17.

Table 17. Sizing of PSV on T-1301.

Variable	Unit	Value
Required area	cm ²	131
Listed area	cm ²	168 (Tipo T)
Discharge flow rate	Nm ³ /h	44587
Size	inch	8 x 10
Rating	-	300 x 150
Model	-	3-5211

6. PROCESS OPTIMIZATION

The optimization of the production process has been carried out by means of the optimal Near equipment where what is done is the cost-based optimization of the different units of the production process.

Optimization of the columns and their operation has been performed as described in section 5.4 based on heuristics that say that the optimum reflux is around 1.2 to 1.5 times the minimum reflux (or 1.1-1.2 times for refrigerated systems).

In this section, the aim is to carry out the cost-based optimization of the T-401 column in order to corroborate the heuristic and the design.

To carry out the optimization based on cost, the equations given by Douglas³⁴ and Turton et al³⁵ have been followed. The price obtained in the equations is described in dollars and is for carbon steel equipment at moderate pressure.

In the case of a complete economic study, the values obtained from the equations described in the bibliography must be adjusted to the current price by means of a correction factor. As in this case, only the cost of different equipment is compared between them, so this factor can be neglected.

Equation 27 describes the cost of the Vessels, this also includes the columns, which is a function of the diameter and height of the equipment, in meters.

$$\text{Cost(\$)} = 17640 \cdot D^{1.066} \cdot L^{0.802} \quad (27)$$

Equation 28 describes the cost of the heat exchanger, which is a function of the exchange area in square meters.

$$\text{Cost(\$)} = 7296 \cdot A^{0.65} \quad (28)$$

Equation 29 describes the cost of compressors, given in horsepower (hp).

$$\text{Cost(\$)} = \frac{1293 \cdot 517.3 \cdot 3.11 \cdot \text{hp}^{0.82}}{280} \quad (29)$$

The cost of the utilities is described according to the type of steam, electricity (E) or refrigerant used, as each one has an associated cost, Low-pressure steam (LP), Medium-pressure steam (MP) or high-pressure steam (HP), in the case of refrigerant, only the use of water (Wr) is considered to be associated with the condenser.

$$\text{Cost(\$)} = 7.78 \cdot LP + 8.22 \cdot MP + 9.88 \cdot HP + 16.8 \cdot El + 4.43 \cdot Wr \quad (30)$$

A Visual Basic Excel code has been created that is able to take data from the number of stages and the feeding stage and automatically obtain the values of diameter and height from Aspen Plus, for these values it is necessary that the column internals, steam consumption and coolant consumption are activated.

In the case of the distillation column, Aspen does not provide the calculation of the necessary exchange area in the reboiler and condenser, so it is necessary to estimate this value from the heat given in this unit, the logarithmic temperature difference and the overall heat transfer coefficient using Equation 31.²⁹

$$Q = U \cdot A \cdot \Delta T_{LM} \quad (31)$$

The value of the heat transfer coefficient is obtained from literature where for the condenser it is 490 kcal/(h m²K) and for the reboiler it is 730 kcal/(hr m²K).³⁶

The VISUAL BASIC code used is shown in Appendix 8.

In the case of the T-401 column, it is already known that the steam used is medium pressure and that the calculation is made with refrigerant, as it is easier to approximate. The values obtained from the scan for the optimization are shown in Figure 23, where it can be seen that the optimum point for the number of trays and feed stage is shown in Table 18.

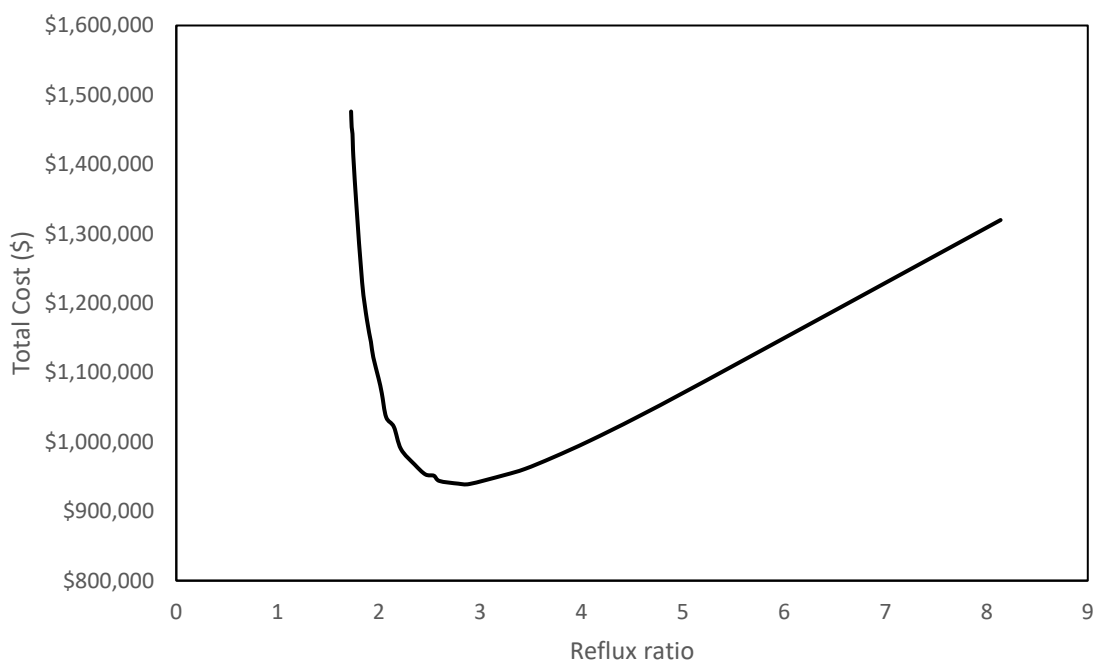


Figure 23. Total Cost of equipment vs reflux ratio.

Table 18. Optimum result of the distillation column T-401.

N° Stage	Feed stage	Column Cost	Reboiler Cost	Condenser Cost	Utility Cost	Total Cost
42	23	9.36E+05	1.75E+03	1.11E+03	5.97E+02	9.39E+05

Comparing the value obtained with the heuristic, it is observed that it provides a correct and optimum value to the process, thus validating the procedure described and designing the optimum of the individual equipment.

7. ECONOMIC EVALUATION

In order to study the economic feasibility of the project, the Equipment Costs methodology is used.³⁷

7.1 Calculation of initial investment

The Equation 32 is used to obtain the initial investment of the equipment.

$$Cost_e = a + bS^n \quad (32)$$

Where a and b are constants unique to each device, S is the size parameter (depending on each device) and n is the characteristic exponent of each device, the Tables with the constants, as well as the values of S and n are shown in Appendix 8.

The values obtained through the equation describe the price of the equipment in 2010, so the price of the equipment must be updated by means of a correction factor that is calculated with the CEPCI between the current year and 2010, the bibliographic reference value.³⁸

On the other hand, the cost of the installation of the equipment has to be taken into account, this factor depends on each equipment, the tabulated value is shown in Appendix 9.

Finally, it is necessary to consider the material factor of the equipment, being a value of 1 for carbon steel materials and 1.3 for stainless steel materials.

The equation with the correction factors results in Equation 33.

$$Cost = C_e \cdot \frac{CEPCI_{2022}}{CEPCI_{2010}} \cdot f_i \cdot f_m \quad (33)$$

The total investment of the new unit where the equipment, valves and pipes of the project are taken into account is 56,934,179.76 €.

Obtaining a total investment including the reference project of 107,993,589.78 €.

7.2 Feasibility study

After calculating the initial investment, the feasibility of the project is calculated using the Net Present Value (NPV) and the Payback.

To do so, the income and losses of the production process are calculated using Equations 34 and 35.

$$Income \left(\frac{\text{€}}{\text{year}} \right) = \sum W_{p,i} Pr_i \quad (34)$$

$$Losses \left(\frac{\text{€}}{\text{year}} \right) = \sum W_{r,i} Pr_i + \sum \text{utilities } Pr_i + \sum n^o \text{ workers} \cdot \text{Salary} \quad (35)$$

Depreciation is calculated assuming a useful life of the equipment of 20 years and a residual value of 0 that show in the Equation 36.

$$\text{Depreciation} = \frac{\text{Initial investment} - \text{Residual value}}{\text{Lifetime}} \quad (36)$$

Subsequently, the profit before tax and the profit after tax are calculated considering a rate of 35% (t).

$$B.A.I = \text{Income} - \text{Losses} - \text{Depreciation} \quad (37)$$

$$B.D.I = (1 - t)BAI \quad (38)$$

The Cash Flow (CF) of the investment is calculated using Equation 39.

$$CF = B.D.I + \text{Depreciation} \quad (39)$$

Finally, the NPV is calculated with a rate of return of 12%, payback and IRR from the Equations 40 and 41.

$$NVP = -I_o + \sum \frac{CF}{(1+i)^n} \quad (40)$$

$$\text{Payback} = \frac{\text{initial Investment}}{\text{Cash Flow}} \quad (41)$$

Table 19. Summary of the economic evaluation.

	<i>Cost</i>
Initial investment (M€)	108
Profit (M€)	391
- benzene	91.2
- p-xylene	256.3
- others	43.2
- gases	4.0
Losses (M€)	337
- raw materials	293
- energy	43.9
- workers	0.4

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Depreciation (M€)	3
B.A.I (M€)	48.5
Corporate tax (M€)	17.0
B.D.I (M€)	31.6
<i>Cash Flow</i> (M€)	37.0
NVP (M€)	25.2
<i>Payback</i> (year)	3
IRR	0.21

As can be observed in the table above, at 5 years a positive NPV is obtained, making the project viable, in addition to recovering the money in a total of 3 years.

It should be noted that these values are subject to change depending on the prices of the raw materials and products obtained.

8. CONCLUSIONS

After the execution of the project to achieve the production of p-xylene and benzene by disproportionation of toluene, the following conclusions are drawn:

- Currently, the most used technology on the market and the one implemented in the project is the purification of p-xylene by continuous adsorption. On the other hand, it has been found that for the isomerization reaction a catalyst is being developed with the capacity to generate more p-xylene instead of ethylbenzene dealkylation, a useful study if the demand for benzene decreases and it is not necessary to obtain it.
- The synthesis of the production process has been developed to obtain two products, p-xylene with a purity of 99.4 % and a purity for benzene of 99.5 %.
- Simulation of the production process was carried out using Aspen Plus v.12 and used to characterize the operating conditions and equipment dimensions. In addition to obtaining the material and energy balance of the different sections.
- The individual optimization of the equipment has been carried out in order to obtain a process close to the optimum, corroborating the heuristic that the reflux that minimizes the total price of the equipment is between 1.2- 1.5 of the minimum reflux in the distillation columns.
- It has been obtained that the project has a value of 108M€ including the installation of the reference project and the one developed in this document. To see the viability of the project, the current market has been considered, if the price of raw materials, products and their demand remains constant, and an IRR of 21.1 % and an NPV of 25.2 M€ over a period of 5 years has been obtained. In addition, the pay-back of the process is 3 years.

9. NOTATION

A	Area m^2	$Pdch$	Pressure discharge Pa
Ad	Simulated flow rate of the pore volume of selective adsorbent m^3h^{-1}	Pr	Price €
CA	Corrosion over-thickness mm	PUX	Purity of p-xylene
C_e	Cost equipment €	Q	Heat quantity kW
D	Diameter m	r	Radius m
E	Welding efficiency	R	Resistance of heat transfer $W m^{-1}$
El	Energy by Electricity MGj	REC	Recovery factor of p-xylene
E	Extract	Re	Reynolds
F	Feed	S	Allowable stress kPa
f	Friction factor	T	Temperature K
f_i	Instalation factor	U	Heat transfer coefficient $kcal/h m^{-1}K^{-1}$
f_m	Material factor	u_t	liquid deposition rate $m s^{-1}$
G	Gravity acceleration $m s^{-2}$	v	Velocity $m s^{-1}$
H	Enthalpy kJ/mol	V'	Volumetric flow $m^3 s^{-1}$
h_b	Head of the bomb m	W	mass flow $kg h^{-1}$
hf	Pressure drop m	x_i	Molar composition
h_m	Minor pressure drop m	Z	Comprehensibility coefficient
hp	Power hp	ΔT_{LM}	Logarithmic temperature difference
HP	Energy by High-pressure MGj	ϵ	Rugosity
h_i	Heat transport coefficient $W m^{-1} k^{-1}$	ϵ	Porosity
K	Corrector coefficient	ρ	Density $kg m^{-3}$
kp	Presure drop coeficient	μ	kinematic viscosity $m^2 s^{-1}$
k_i	Thermal conductivity of the material $W m^{-1} k^{-1}$	t	Thickness mm
L	Length m	t^*	Switching time s^{-1}
LP	Energy by Low-pressure MGj	t_c	Cycle time s^{-1}
M	Molar mass $kg mol^{-1}$		
MP	Energy by Mid-pressure MGj		
m^{total}	Total mass kg	CAGR	Compound Annual Growth Rate
P	Pressure Pa	NPV	Net Present Value
Pdi	Pressure design kPa	IRR	Internal Rate of Return

10. REFERENCES AND NOTES

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APPENDIX

APPENDIX 1: P&ID

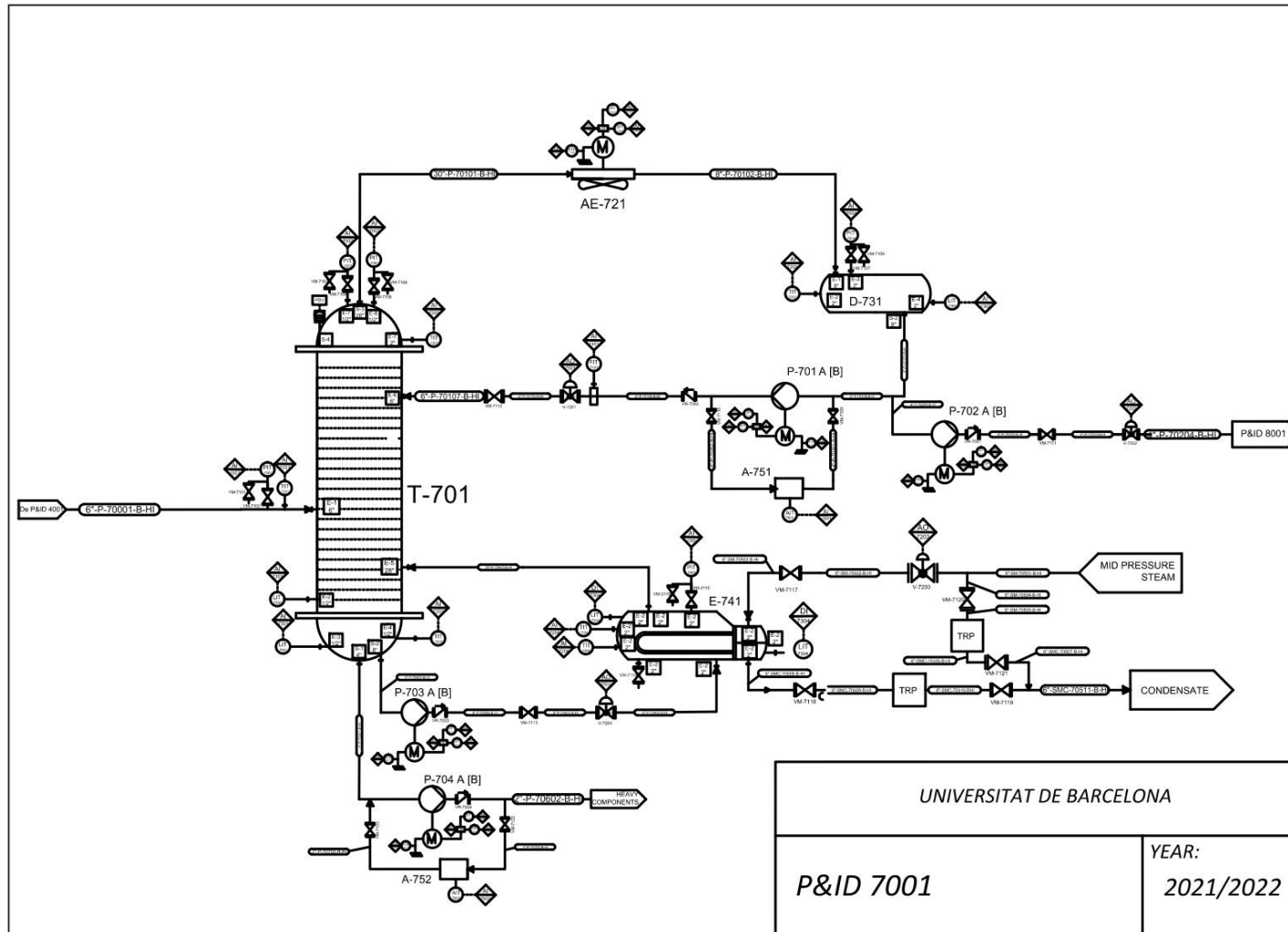


Figure 24. P&ID 7001

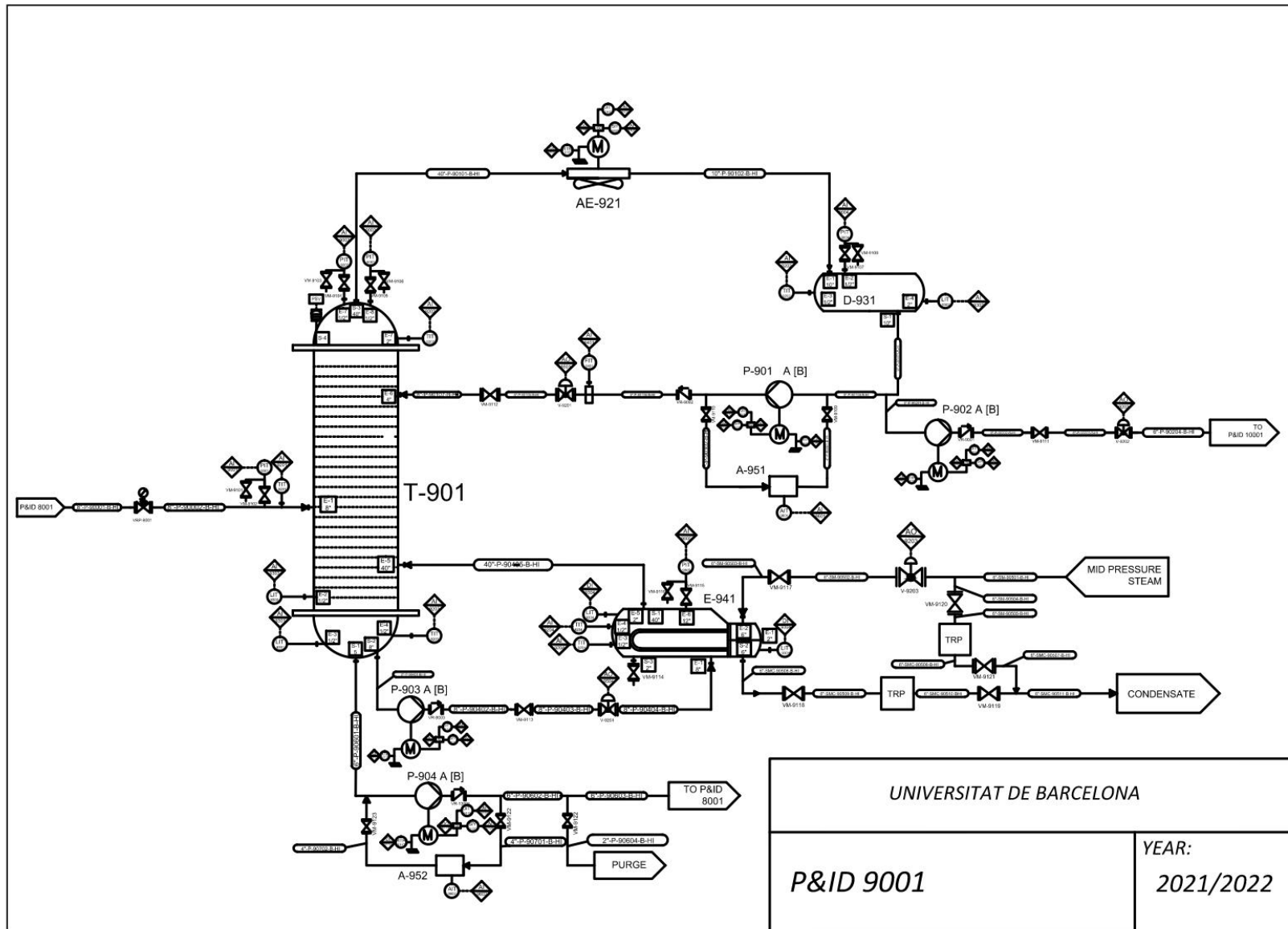


Figure 25. P&ID 9001

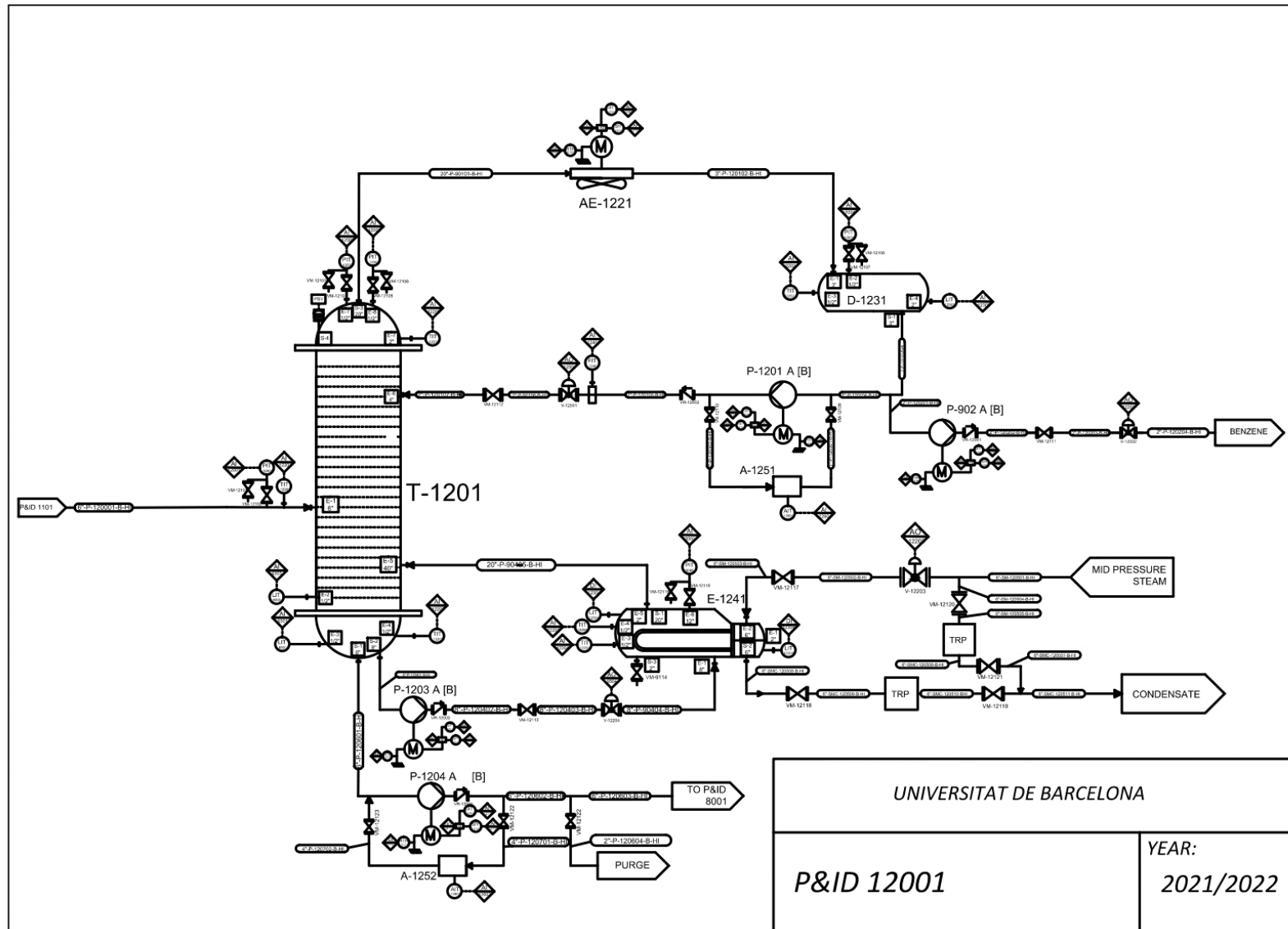


Figure 26. P&ID 12001

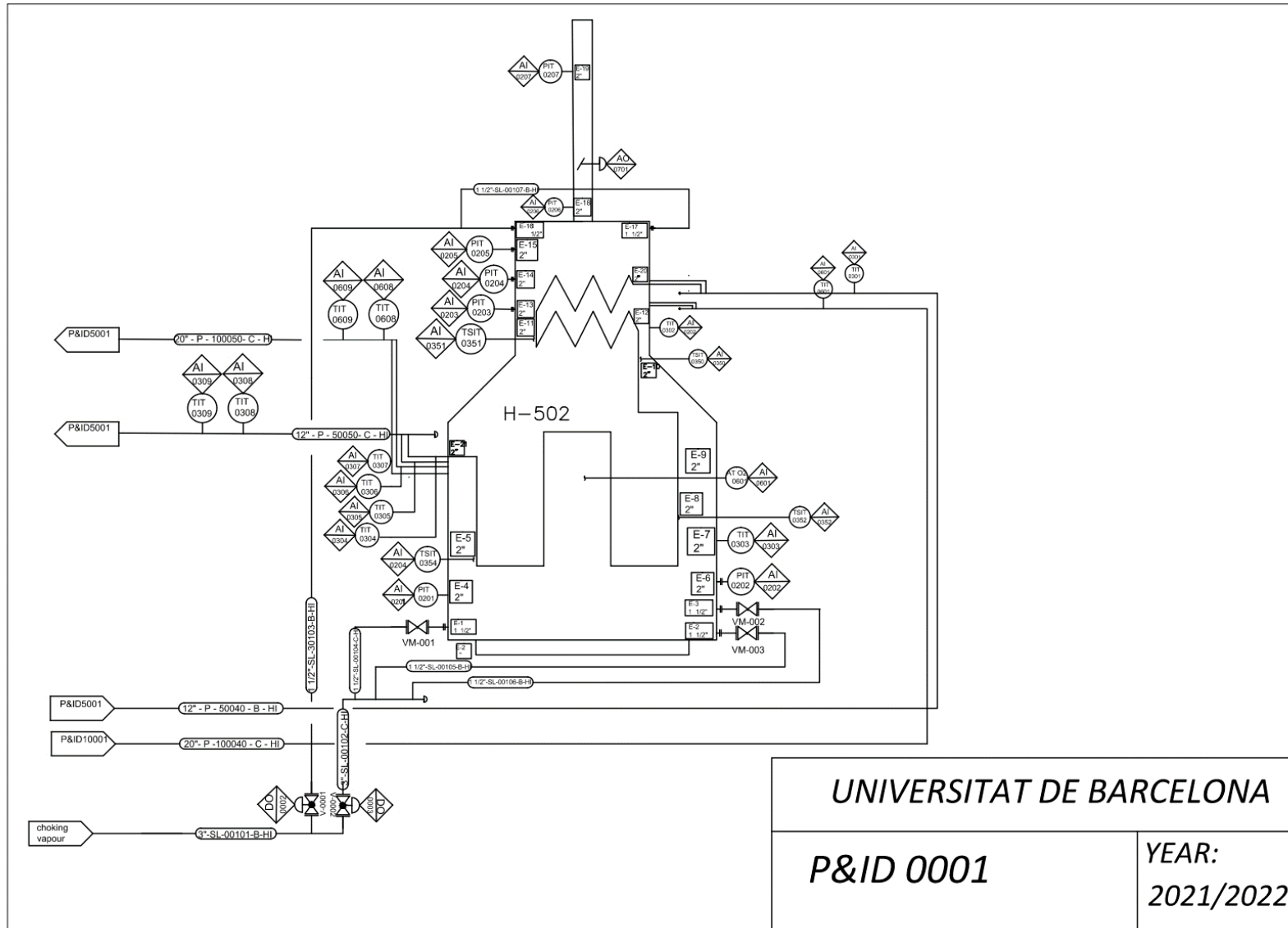


Figure 27. P&ID 12001





P&ID Symbology	Description	
<p><i>AX</i></p> <p><i>DX</i></p>    	<p>Analogue Transmitter</p> <p>Digital Transmitter</p> <p>Control valve</p> <p>Manual Valve</p> <p>Check valve</p> <p>Steam tramp</p>	<p>Diameter of pipe</p> <p>Line type (P: Process, SH: High Steam, SL: Low Steam, SHC: SH condensate, SLC: SL condensate). of SH, SLC: Condensate of SL)</p> <p>X" - X - XXXXX - X - XX</p> <p>Pipe line</p> <p>Line conditions: HI: Heat Insulated HT: Heat Traced</p> <p>Pipe specification: B: Carbon steel grade B C: H316L stainless steel P91: Alloy steel A335 grade P91</p>
		<p>UNIVERSIDAD DE BARCELONA</p>
		<p><i>P&ID Symbology</i></p>
		<p>2021/2022</p>

Figure 28. P&ID SYMBOLOGY

APPENDIX 2: INTERNAL SIZING OF DISTILLATION COLUMN.

Once the number of trays, reflux and feed stage have been characterized, the internal design of the column is carried out using Aspen Plus.

To do this, it is necessary to enter the column to be characterized and use the tool described as Internals, within the interface the automatic selection is made by fluid inlet and outlet locations, characterizing the column in two as shown in the following Figure 29.

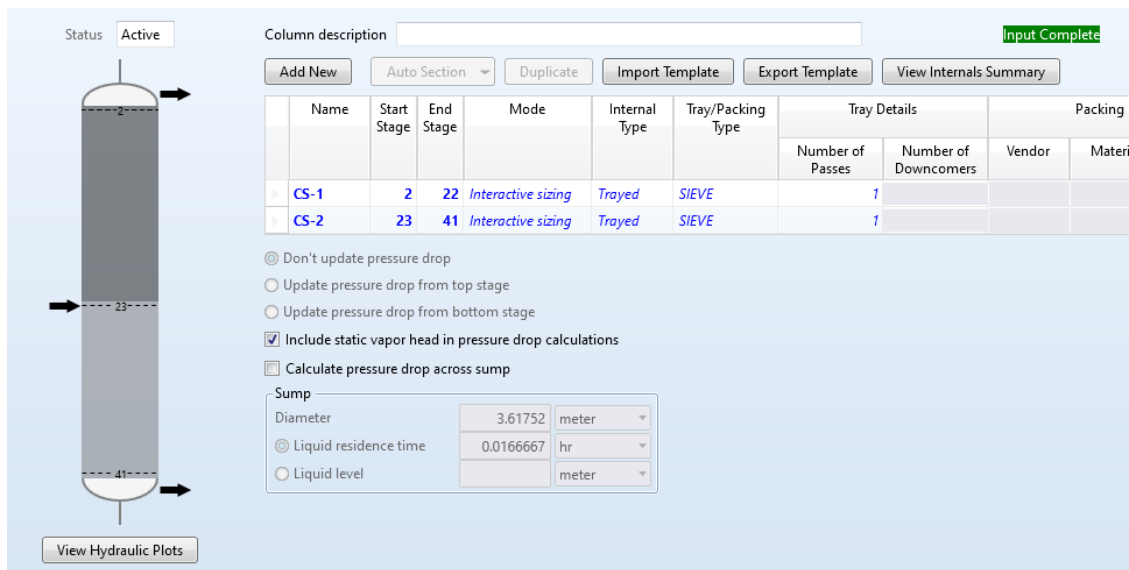


Figure 29 Configuration of the internal column.

After the first sizing is done, with the interactive sizing model, the first values are obtained. As can be seen, the difference between the diameters is smaller than 0.2 meters, so the diameter of the column is modified to the highest value.

After modification, the interface marked as "View hydraulic plots" is entered in order to see the internal operation of the column plates and that there is no warning of the operation.

In this interface we have elements that are necessary to analyze for the correct operation of the column.

On the left side of the interface and as shown in the following figure, the general scheme of the simulation of the column is shown, in this scheme there are three colors, Blue, correct operation, Yellow: Warning for some reason, Red, error in the simulation of the trays. That show in the Figure 30.

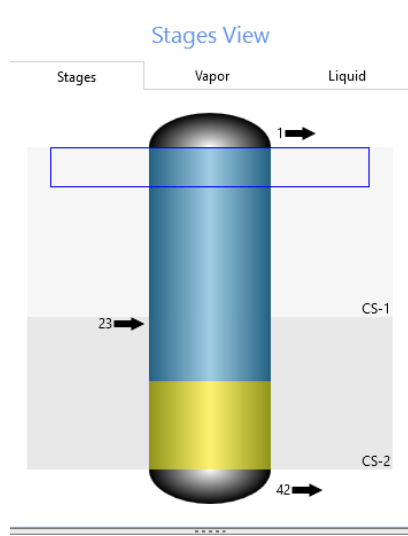


Figure 30. Representation of the interface.

The right-hand side of the interface shows the operating diagram of the column plate and the interface for moving between the different trays, in order to visually check that you are working within the required area, as shown in Figure 31.

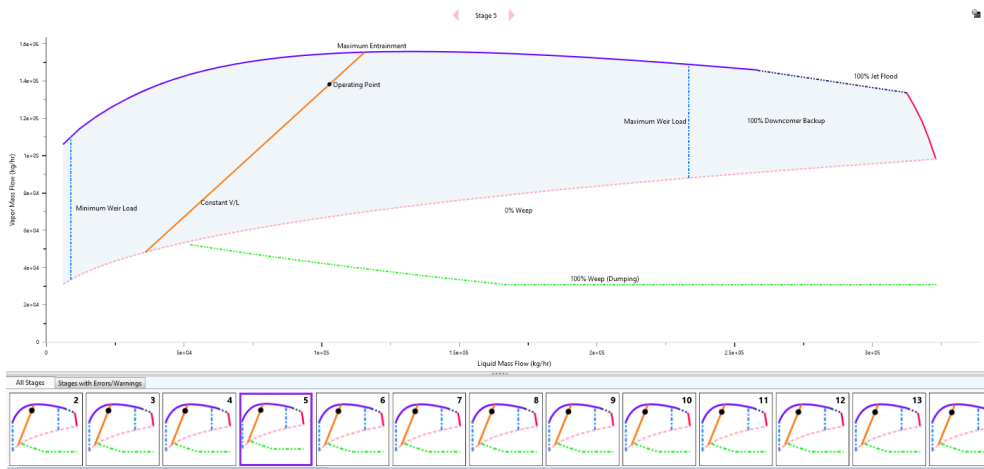


Figure 31. Representation of operating diagram tray.

Finally, the lower left corner describes the Downcomer Loading relative to the Choke Flood of the scenario and the Weir Loading.

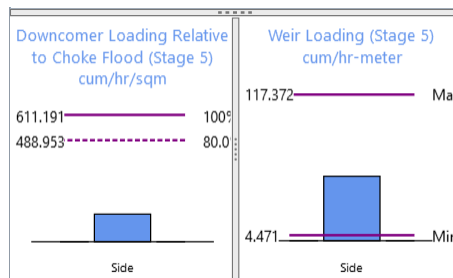


Figure 32. Lower left corner interface.

As can be seen in Figure 30, the column used to explain the resolution and verification procedure presents certain Warnings in the trays at the bottom of the column.

To do this, it is necessary to enter the plate and analyze the warning of the program as shown in the Figure 33.

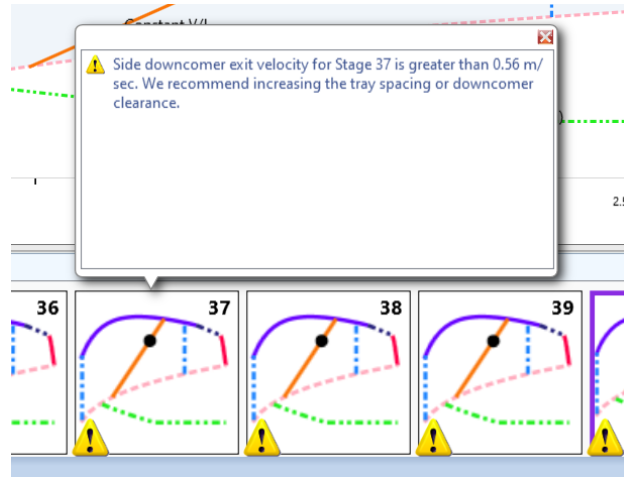


Figure 33. Warning of the trays at the bottom.

Where it specifies that it is necessary to modify certain parameters of the column so that it operates correctly within the established margins. Such as the downcomer clearance or the height between trays. In this case, the spacing between plates is modified with small increments in order to obtain the correct operation of the column, showing the final result of the column as shown in Figure 34.

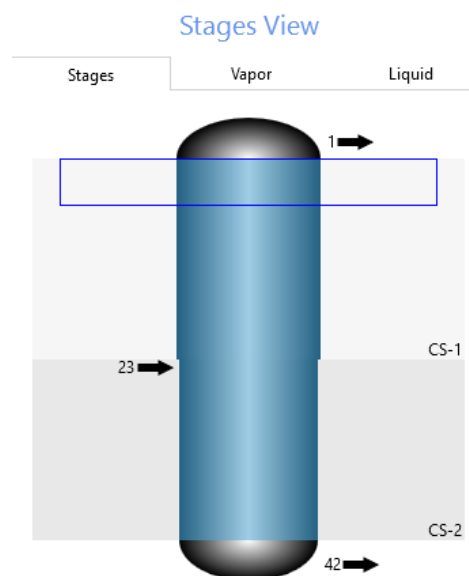


Figure 34. Correct result of the internal design.

APPENDIX 3: ADSORPTION COLUMN

Resolution Material balance adsorption column

To solve the material balance in the adsorption column, the first step is to know the total flow rate of p-xylene obtained by the extract and in turn to define the flow rate of p-xylene lost by the extract, this is done by the Equations 44 and 45.

$$F \cdot x_{p-x}^f \cdot REC = E \cdot x_{p-x}^E \quad (44)$$

$$F \cdot x_{p-x}^f = E \cdot x_{p-x}^E + R \cdot x_{p-x}^R \quad (45)$$

Subsequently, a hypothetical flow rate (HR) is made which describes the refining flow rate without taking into account the desorbent, Equation 46.

$$HR = \frac{E \cdot x_{p-x}^E}{PUX} \quad (46)$$

The mole fraction of para xylene in the extract is determined because values have been obtained in the bibliography both on an industrial scale and in the simulation of this value. The value of the desorbent flow rate is obtained with the following Equation 47.

$$D^E = E - HR \quad (47)$$

And considering that the composition of the rest of the main compounds in the stream depends on the composition of the inlet flow, it is solved by the following Equations 48, 49, 50 and 51.

$$S = F \cdot x_{o-x}^f + F \cdot x_{m-x}^f + F \cdot x_{EB}^f \quad (48)$$

$$E \cdot x_{o-x}^E = (HR - E \cdot x_{p-x}^E) \cdot \frac{F \cdot x_{o-x}^f}{S} \quad (49)$$

$$E \cdot x_{m-x}^E = (HR - E \cdot x_{p-x}^E) \cdot \frac{F \cdot x_{m-x}^f}{S} \quad (50)$$

$$E \cdot x_{EB}^E = (HR - E \cdot x_{p-x}^E) \cdot \frac{F \cdot x_{EB}^f}{S} \quad (51)$$

After the flow rate is known, the material balances for all the species are solved, considering that all the species that have not been named in the extract have a value of 0.

$$F \cdot x_i^f = E \cdot x_i^E + R \cdot x_i^R \quad (52)$$

To determine the final desorbent flow rate, the mole fraction of the desorbent is marked and the value is obtained, using Equations 53 and 54.

$$D^R = R \cdot x_D^R \quad (53)$$

$$D = D^E + D^R \quad (54)$$

Operational parameters¹⁰

Having the material balance and knowing the inlet flow rate, the first step is to use the value of the aromatic feed flow rate to determine the necessary simulated flow rate of the pore volume of the selective adsorbent to achieve an effective separation. Using Equation 55.

$$Ad = \left(\frac{Ad}{V_F^{la}} \right) \cdot V_F^{la} = \varepsilon_\mu \cdot V_{solido}^{TMB} \quad (55)$$

Where the variable $\left(\frac{Ad}{V_F^{la}} \right)$ describes the simulated solid velocity and the liquid velocity, this value can vary in the range of 0.69 and 0.71. The value of the required adsorbent flow rate can be known directly.

Knowing the required adsorbent flow rate, the value of the selective volume is obtained by means of the correlation that show in Equation 56.

$$V_s = -0.0092 \cdot Ad + 1.3345 \quad (56)$$

Subsequently the cycle time is calculated using Equation 57

$$t_c = \frac{V_s}{Ad} \quad (57)$$

And once the cycle time is known, the switching time of the ports is calculated, this is done by dividing the cycle time by the number of chambers, industrially a value of 24, as shown in Equation 58.

$$t^* = \frac{t_c}{24} \quad (58)$$

This switching time is used to calculate the inlet and outlet flow rates for cleaning and recycling, Equation 59 and 60.


$$Q_H = \frac{f_H^{line} \cdot v_{line}}{t^*} \quad (59)$$

$$Q_X = \frac{f_X^{line} \cdot v_{line}}{t^*} \quad (60)$$

This defines both the dimensioning of the column, due to the values of the selective volume, and its operation. Once these points are known, it is possible to know the internal flow rates as described in the reference article.

APPENDIX 4: HEAD EXCHANGER DATA SHEET

Heat Exchanger Specification Sheet

1	Company:											
2	Location:											
3	Service of Unit:					Our Reference:						
4	Item No.:					Your Reference:						
5	Date:		Rev No.:			Job No.:						
6	Size: 675 - 4950		mm		Type: BEM		Horizontal		Connected in: 5 parallel 4 series			
7	Surf/unit(eff.)		3209.2		m ²		Shells/unit 20		Surf/shell(eff.) 160.5 m ²			
8	PERFORMANCE OF ONE UNIT											
9	Fluid allocation				Shell Side			Tube Side				
10	Fluid name				P21			P17				
11	Fluid quantity, Total				kg/s 23.7698			23.7698				
12	Vapor (In/Out)		kg/s		23.7698		7.6295		4.1513 23.7698			
13	Liquid		kg/s		0		16.1403		19.6185 0			
14	Noncondensable		kg/s		0		0		0 0			
15												
16	Temperature (In/Out)				°C 420		122.91		97.82 379.76			
17	Bubble / Dew point				°C -175.55 / 173.82		-177.54 / 172.72		31.23 / 176.54 26.77 / 176			
18	Density Vapor/Liquid		kg/m ³		5.47 /		3.75 / 768.31		2.37 / 795.93 5.74 /			
19	Viscosity				mPa-s 0.0181 /		0.0126 / 0.2322		0.0119 / 0.2865 0.0172 /			
20	Molecular wt, Vap				31.52		12.78		7.34 31.52			
21	Molecular wt, NC											
22	Specific heat		kJ/(kg-K)		2.979 /		3.4 / 2.094		4.85 / 2.003 2.901 /			
23	Thermal conductivity				W/(m-K) 0.147 /		0.1338 / 0.1067		0.1576 / 0.1126 0.14 /			
24	Latent heat				kJ/kg 314.9		345.6		354.2 314.2			
25	Pressure (abs)				bar 10		9.74513		10 9.87539			
26	Velocity (Mean/Max)				m/s 5.52 / 8.21				5.18 / 8.63			
27	Pressure drop, allow./calc.				bar 0.26		0.25486		0.5 0.12461			
28	Fouling resistance (min)				m ² -K/W 0				0 0 Ao based			
29	Heat exchanged		23952.9		kW		MTD (corrected) 24.89		°C			
30	Transfer rate, Service		299.9		Dirty 334.1		Clean 334.1		W/(m ² -K)			
31	CONSTRUCTION OF ONE SHELL								Sketch			
32					Shell Side		Tube Side					
33	Design/Vacuum/test pressure		bar 11 / /		11 / /							
34	Design temperature / MDMT		°C 455 /		455 /							
35	Number passes per shell				1		1					
36	Corrosion allowance				mm 3.18		3.18					
37	Connections		In mm 1 355.6 / -		1 203.2 / -							
38	Size/Rating		Out 1 304.8 / -		1 203.2 / -							
39	Nominal		Intermediate 1 304.8 / -		1 203.2 / -							
40	Tube #: 555 OD: 19.05 Tks. Average 2.11 mm Length: 4950 mm Pitch: 23.81 mm Tube pattern:30											
41	Tube type: Plain Insert:None Fin#: #/m Material:Carbon Steel											
42	Shell Carbon Steel		ID 675 OD 697		mm		Shell cover -					
43	Channel or bonnet Carbon Steel						Channel cover -					
44	Tubesheet-stationary Carbon Steel -						Tubesheet-floating -					
45	Floating head cover -						Impingement protection None					
46	Baffle-cross Carbon Steel		Type Single segmental		Cut(%d) 40.83		Hori Spacing: c/c 585		mm			
47	Baffle-long - Seal Type						Inlet 952.98		mm			
48	Supports-tube U-bend		0		Type							
49	Bypass seal Tube-tubesheet joint Expanded only (2 grooves)(App.A 'i')											
50	Expansion joint - Type None											
51	RhoV2-Inlet nozzle 522		Bundle entrance 218		Bundle exit 217		kg/(m-s ²)					
52	Gaskets - Shell side -				Tube side		Flat Metal Jacket Fibe					
53	Floating head -											
54	Code requirements ASME Code Sec VIII Div 1				TEMA class R - refinery service							
55	Weight/Shell 4440.2		Filled with water 6201		Bundle 2807		kg					
56	Remarks											
57												
58												

APPENDIX 5: PRESURE DROP IN PIPELINE

The pressure drop in the pipes has been determined considering one meter of pipe and knowing the roughness of the pipe (ϵ), being a value of 4.5 millimeters.

The pressure drop in pipes occurs for two reasons:

- In straight pipes, caused by the roughness of the pipe, higher losses.
- Fittings that are implemented to the pipe, such as elbows, valves, minor losses.

Major losses

To determine the value of the major losses, value of the loss for a lineal pipe, it is calculated by the Equation 61.

$$h_f = f \cdot \frac{L \cdot v^2}{D \cdot \nu_{isc}} \quad (61)$$

Where the friction factor can be obtained from certain correlations, in this case it is decided to use Swanee and Jain (1976), Equation 62, Haaland (1983), Equation 63, and the correlation of the Darcy factor, Equation 64.

$$f = \frac{0.25}{\left[\log \left(\frac{\epsilon}{3.7} + \frac{5.74}{Re^{0.9}} \right) \right]^2} \quad (62)$$

$$\frac{1}{\sqrt{f}} = -1.8 \cdot \log \left(\frac{\epsilon}{3.7} + \frac{6.9}{Re} \right) \quad (63)$$

$$A = \left(2,457 \ln \left(\frac{1}{\left(\frac{7}{Re} \right)^{0.9} + 0,27 \frac{\epsilon}{D}} \right) \right)^{16} \quad B = \left(\frac{37530}{Re} \right)^{16} \quad f = 8 \left(\left(\frac{8}{Re} \right) + \frac{1}{(A+B)^{1,5}} \right)^{1/12} \quad (64)$$

It is necessary to check that the fluid is in a turbulent state in order to be able to apply the above equations, this is done from the Reynolds, Equation 65.

$$Re = D \cdot v \cdot \rho / \mu \quad (65)$$

Minor losses

Minor losses can be calculated in different methods.

The first is from the pressure loss coefficient (k_p) provided by the manufacturer, in order to obtain the pressure drop in meters, by the Equation 66.

If this value is to be estimated without taking the manufacturer into account, there are bibliographic data that show an approximation of the value of k_p .

$$h_m = k_p \cdot \frac{v^2}{2 \cdot g} \quad (66)$$

The second way is through the equivalent length. The equivalent length (Le) term and using the Equation 67. Bibliographic data from Le/D show in Table 20.

$$h_m = f \cdot \frac{Le}{D} \cdot \frac{v^2}{2 \cdot g} \quad (67)$$

Table 20. Le/D ratio according to the type of accessory.

Type of accessory	Le/D
Seat	450
Globe - Fully open	340
Angular - Fully open	150
Gate - Full Open	8
Gate - 1/4 open	900
Gate - 2/4 open	160
Gate - 3/4 open	35
Ball - Full Open	20
Check	100
Check - Valve	150
Butterfly - Full Open or (2 to 8 in.)	45
10 to 14 in.	35
16 to 24 in.	25
Foot Valve - Stem Disc Valve	420
Hinged Disc Foot Valve	75
Standard 90° Elbow	30
Long Radius 90° Elbow	20
90° Threaded Elbow	50
45° Standard Elbow	16
45° threaded elbow	26
Closed loop on return	50
Standard tee with direct flow	20
With flow in the branch	60
Tank inlet	50
Tank outlet	25

There is another way, in the case of pipes with a certain length, and that is to make the approximation that the pressure loss through the fittings is about 30% of the major losses of the pipe.

APPENDIX 6: List of piping

Table 21. List of piping

N° PFD	N° P&ID	diameter (inch)	T (°C)	P. op. (bar a)	Td (°C)	Pd (bar a)	Velocity (m/s)	Di (mm)	Thickness (mm)	Model	Pressure drop (cm /m pipe)			Insulate thiknes (mm)	
											SyJ	H	D		
16	12''-P70002-B-HI	12.00	148	1.16	173.41	1.31	3.75	305	9.53	Std 40	2.87	2.86	3.00	14.9	30
17	4''-P70204-B-HI	4.00	138	1.00	163.47	1.29	1.58	102	6.02	Std 40	6.01	5.99	4.32	12.2	30
19	2''-P70602-B-HI	2.00	176	1.29	200.68	1.33	1.65	53	3.91	Std 40	14.57	14.52	14.41	17.2	30
44	4''-P80001-B-HI	4.00	139	9.00	164.03	2.43	1.58	102	6.02	Std 40	6.01	6.00	0.35	12.3	30
45	6''-P80002-B-HI	6.00	142	9.00	167.25	2.43	2.07	154	7.11	Std 40	5.56	5.54	1.62	13.3	30
46	6''-P80003-B-HI	6.00	173	9.00	198.00	2.43	2.16	154	7.11	Std 40	5.79	5.77	2.55	19.0	30
47	8''-P80101-B-HI	8.00	173	9.00	198.00	2.43	0.74	307	8.18	Std 40	0.40	0.40	0.04	19.9	30
50	6''-P130001-B-HI	6.00	173	9.00	198.00	2.43	0.42	310	7.11	Std 40	0.15	0.14	0.01	19.9	30
51	8''-P130002-B-HI	18.00	164	1.07	189.15	1.30	3.12	429	14.3	Std 40	3.22	3.21	0.98	18.3	30
52	4''-P130204-B-HI	4.00	138	1.00	162.95	1.29	1.20	102	6.02	Std 40	3.73	3.72	0.12	12.2	30
54	6''-P130602-B-HI	6.00	189	1.15	213.71	1.31	1.66	128	6.55	Std 40	4.80	4.79	0.55	21.9	30
57	8''-P90001-B-HI	8.00	173	9.00	198.00	2.43	1.99	203	8.18	Std 40	3.64	3.63	1.88	19.4	30
58	8''-P90002-B-HI	8.00	159	1.11	183.74	1.30	1.75	203	8.18	Std 40	2.97	2.96	0.98	16.5	30
59/60	6''-P90602-B-HI	6.00	189	1.15	213.92	1.31	4.24	102	7.11	Std 40	32.42	32.33	18.82	21.4	30
63	6''-P90204-B-HI	6.00	137	5.20	162.01	1.89	1.52	154	7.11	Std 40	3.31	3.30	0.44	12.4	30
64	6''-P100020-C-HI	6.00	138	1.77	162.53	1.40	1.52	154	7.11	Std 40	3.31	3.30	0.45	12.5	30
65	26''-P100030-C-HI	26.00	98	6.60	122.82	2.09	5.50	641	9.53	Std 40	5.61	5.60	1.36	6.6	30
66	20''-P100040-C-HI	20.00	380	5.91	405.00	1.99	21.77	489	9.53	Std 40	43.22	42.83	36.17	97.4	100
67	20''-P100050-C-HI	20.00	420	2.14	445.00	1.45	23.13	489	9.53	Std 40	2.49	2.46	2.08	120.0	120
-	20''-P100050-C-HI	3.00	183	2.14	445.00	1.45	1.29	78	5.49	Std 40	3.25	3.22	2.72	30.0	30

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68	20''-P100060-C-HI	20.00	420	1.62	445.00	1.37	23.13	489	9.53	Std 40	3.70	3.66	3.09	120.0	120
69	16''-P100060-C-HI	16.00	123	40.0	148.32	6.86	9.57	514	22.23	60	19.08	19.04	6.31	10.6	30
70	16''-P100070-C	16.00	32	40.0	57.00	6.86	4.74	616	22.23	60	5.05	5.04	1.09	0.0	30
71	12''-P100090-C	12.00	32	40.0	57.00	6.86	20.27	295	14.28	60	6.42	6.40	1.38	0.0	30
72	4''-P100100-C	4.00	32	40.0	57.00	6.86	16.91	102	6.02	Std 40	3.59	3.58	0.77	0.0	30
73/74	10''-P100090-C	10.00	32	40.0	57.00	6.86	24.56	255	9.27	Std 40	4.68	4.67	1.01	0.0	30
75	5''-P100120-C	5.00	32	40.0	57.00	6.86	14.17	128	6.55	Std 40	3.12	3.11	0.67	0.0	30
76	10''-P100130-C	10.00	32	40.0	56.98	6.86	28.16	255	9.27	Std 40	5.14	5.13	1.11	0.0	30
78	5''-P10080-C	5.00	32	40.0	57.00	6.86	1.93	128	6.55	Std 40	7.69	7.66	0.24	0.0	30
79	6''-P110204-B-HI	2.00	32	40.0	57.00	6.86	18.38	35	12.70	Std 40	6.45	6.43	0.20	0.0	30
81	6''-P120001-B-HI	6.00	32	40.0	57.42	6.86	1.52	143	12.70	Std 40	4.59	4.58	0.09	0.0	30
82	2''-P120204-B-HI	2.00	80	40.0	104.81	6.86	0.68	49	5.54	XS 80	4.44	4.42	0.06	3.8	30
83	6''-P120601-B-HI	6.00	143	40.0	168.42	6.86	1.41	154	7.11	Std 40	2.87	2.86	0.36	13.5	30
84	6''-P120602-B-HI	6.00	144	40.0	168.89	6.86	1.41	154	7.11	Std 40	2.87	2.86	0.36	13.5	30
85	2''-P120604-B-HI	2.00	144	40.0	168.89	6.86	0.41	49	5.54	XS 80	1.77	1.76	0.03	12.2	30
86	6''-P120603-B-HI	6.00	144	40.0	168.89	6.86	1.37	154	7.11	Std 40	2.72	2.72	0.32	13.5	30
	30''-P70101-B-HI	30.00	140	1.00	165.00	1.29	27.42	743	9.53	Std 40	5.06	5.05	1.67	13.7	30
	6''-P70106-B-HI	6.00	140	1.00	165.00	1.29	2.02	154	7.11	Std 40	2.53	2.52	0.84	12.9	30
	8''-P130401-B-HI	8.00	168	1.30	193.00	1.33	0.78	307	8.18	Std 40	2.53	2.52	0.84	18.8	30
	30''-P130405-B-HI	30.00	168	1.30	193.00	1.33	21.22	743	9.53	Std 40	3.80	3.79	1.26	19.5	30
	26''-P130101-B-HI	26.00	138	1.00	163.00	1.29	23.12	641	9.53	Std 40	2.53	2.52	0.84	13.7	30
	4''-P130106-B-HI	4.00	138	1.00	163.00	1.29	2.72	102	6.02	Std 40	2.53	2.52	0.84	12.2	30
	28''-P130405-B-HI	26.00	189	1.50	214.00	1.36	19.72	641	9.53	Std 40	5.06	5.05	1.67	24.3	30
	8''-P130401-B-HI	8.00	189	1.50	214.00	1.36	0.70	307	8.18	Std 40	5.06	5.05	1.67	23.5	30
	40''-P90101-B-HI	40.00	137	1.00	162.00	1.29	22.76	997	9.53	Wt.	3.80	3.79	1.26	13.2	30
	8''-P90106-B-HI	8.00	137	1.00	162.00	1.29	0.63	307	8.18	Std 40	3.80	3.79	1.26	12.8	30

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	40''-P90405-B-HI	40.00	190	1.50	215.00	1.36	20.85	997	9.53	Wt.	3.80	3.79	1.26	24.9	30
	8''-P90401-B-HI	8.00	190	1.50	215.00	1.36	0.64	307	8.18	Std 40	2.53	2.52	0.84	23.8	30
	12''-P120101-B-HI	12.00	80	1.00	105.00	1.29	17.63	305	9.53	Std 40	6.33	6.31	2.09	3.8	30
	2''-P120106-B-HI	2.00	80	1.00	105.00	1.29	1.42	53	3.91	Std 40	5.06	5.05	1.67	3.8	30
	20''-P90405-B-HI	20.00	143	1.50	168.00	1.36	24.09	489	9.53	Std 40	6.33	6.31	2.09	14.1	30
	8''-P90401-B-HI	8.00	143	1.50	168.00	1.36	0.66	307	8.18	Std 40	3.80	3.79	1.26	13.9	30
	8''-P70102-B-HI	8.00	140	1.00	165.00	1.29	0.68	307	8.18	Std 40	5.06	5.05	1.67	13.3	30
	8''-P130102-B-HI	8.00	138	1.00	163.00	1.29	0.68	307	8.18	Std 40	6.33	6.31	2.09	13.0	30
	8''-P90102-B-HI	8.00	137	1.00	162.00	1.29	0.76	307	8.18	Std 40	5.06	5.05	1.67	12.8	30
	2''-P120102-B-HI	2.00	80	1.00	105.00	1.29	2.02	53	3.91	Std 40	5.06	5.05	1.67	3.8	30
16	12''-P70002-B-HI	12.00	148	1.16	173.41	1.31	3.75	305	9.53	Std 40	2.87	2.86	3.00	14.9	30

APPENDIX 7: PRESURE RELIEF VALVE (PSV)

The procedure for calculating the flow rate to be relieved in the event of external fire varies depending on whether the interior of the vessel contains a fluid in gas or liquid state, being the gaseous state for the design cases.

The pressure relief setpoint of the safety valve must be marked, as well as the operating temperature and pressure of the equipment. Once this is done, the following equation is used to obtain the temperature at the moment of tripping due to external fire.

$$T_1 = \left(\frac{P_1}{P_n} \right) \cdot T_n \quad (68)$$

Where T1: relief temperature (K), P1: head pressure (bar), Pn: nominal operating pressure (bar), Tn: normal operating temperature (K).

Once the relief temperature has been calculated, the required flow rate is calculated using Equation 69.

$$W = 2.77 \cdot \sqrt{MP_1} \cdot \left[\frac{A' \cdot (T_w - T_1)^{1.25}}{T_1^{1.1506}} \right] \quad (69)$$

The wall temperature of the cases must never exceed 593 °C in the case of carbon steel and 750 °C for stainless steel.

APPENDIX 8: VISUAL BASIC CODE FOR OPTIMIZATION

The code implemented in the column optimization is as follows:

```
Dim nStage As Single, feedStage As Single, columnDiameter As Single,
traySpacing As Single, coldDuty As Single, reflux As Single, heatDuty As
Single, topTemp As Single, bottomTemp As Single

Sub Main_program()
    Call Link_Aspen(nStage, feedStage, columnDiameter, traySpacing,
        coldDuty, reflux, heatDuty, topTemp, bottomTemp)
End Sub

Sub Link_Aspen(nStage, feedStage, columnDiameter, traySpacing, coldDuty,
reflux, heatDuty, topTemp, bottomTemp)

    ' MsgBox ("Starting program")
    ' Setting Asp program path
    Path = Application.ThisWorkbook.Path &
"/Simulación_TFM_xvalldeperéz_FINAL.bkp"

    Set Asp = GetObject(Path)

    Asp.Visible = True
    Asp.SuppressDialogs = True
    Asp.Reinit
    For i = 1 To 32
        nStage = Sheets("HOJA1").Cells(i + 2, 2) ' Trays
        feedStage = Sheets("HOJA1").Cells(i + 2, 3) ' Feed input

        Call ExportData(Path, nStage, feedStage)
        Asp.Engine.Run
        Call ImportData(Path, columnDiameter, traySpacing, coldDuty,
            reflux, heatDuty, topTemp, bottomTemp)
        Sheets("HOJA1").Cells(i + 2, 4) = reflux
        Sheets("HOJA1").Cells(i + 2, 5) = columnDiameter
        Sheets("HOJA1").Cells(i + 2, 6) = traySpacing * nStage
        Sheets("HOJA1").Cells(i + 2, 7) = -heatDuty * 45.849680043192 /
            3041946.65
        Sheets("HOJA1").Cells(i + 2, 8) = -coldDuty * 45.849680043192 /
            3041946.65
        colCost = 17640 * columnDiameter ^ (1.066) * (traySpacing *
            nStage) ^ (0.802) 'One column cost
        AT1 = topTemp - 20
        AT2 = topTemp - 25
        ATLM1 = (AT1 - AT2) / (((Log(AT1 / AT2)) / (Log(2.718282))))
        Area1 = (heatDuty / 1000) / (490 * ATLM1)
        HE1Cost = 7296 * Abs(Area1) ^ (0.65)
        AT1 = Abs(bottomTemp - 250)
        AT2 = Abs(bottomTemp - 245)
        ATLM2 = (AT1 - AT2) / (((Log(AT1 / AT2)) / (Log(2.718282))))
```

```

Area2 = (coldDuty / 1000) / (730 * ATLM2)
HE2Cost = 7296 * Abs(Area2) ^ (0.65)
horsePower = 0
compCost = 1293 * 517.3 * 3.11 * horsePower ^ (0.82) / 280 '
Compressor cost
lpGJ = 0
mpGJ = -heatDuty * 1.50725E-05
hpGJ = 0
electricityGJ = 0
refWaterGJ = -coldDuty * 1.50725E-05

utilityCost = 7.78 * lpGJ + 8.22 * mpGJ + 9.88 * hpGJ + 16.8 *
electricityGJ + 4.43 * refWaterGJ
totalCost = colCost + HE1Cost + HE2Cost + compCost + utilityCost
Sheets("HOJA1").Cells(i + 2, 9) = colCost
Sheets("HOJA1").Cells(i + 2, 10) = HE1Cost
Sheets("HOJA1").Cells(i + 2, 11) = HE2Cost
Sheets("HOJA1").Cells(i + 2, 12) = compCost
Sheets("HOJA1").Cells(i + 2, 13) = utilityCost
Sheets("HOJA1").Cells(i + 2, 14) = totalCost
Next i
End Sub

Sub ExportData(Path, nStage, feedStage)
Set Asp = GetObject(Path)
Asp.Visible = True
Asp.SuppressDialogs = True
Asp.Tree.FindNode("\Data\Blocks\B38\Input\NSTAGE").Value = nStage
Asp.Tree.FindNode("\Data\Blocks\B38\Input\FEED_STAGE\P1").Value =
feedStage
Asp.Tree.FindNode("\Data\Blocks\B38\Input\CA_STAGE2\INT-1\CS-1").Value =
nStage - 2
End Sub

Sub ImportData(Path, columnDiameter, traySpacing, coldDuty, reflux, heatDuty,
topTemp, bottomTemp)
Set Asp = GetObject(Path)
Asp.Visible = True
Asp.SuppressDialogs = True

columnDiameter =
Asp.Tree.FindNode("\Data\Blocks\B38\Output\CA_DIAM6\INT-1\CS-1").Value
traySpacing = Asp.Tree.FindNode("\Data\Blocks\B38\Output\CA_HEIGHT4\INT-
1\CS-1").Value
coldDuty = Asp.Tree.FindNode("\Data\Blocks\B38\Output\COND_DUTY").Value
reflux = Asp.Tree.FindNode("\Data\Blocks\B38\Output\MASS_RR").Value
heatDuty = Asp.Tree.FindNode("\Data\Blocks\B38\Output\DUTY\1").Value
topTemp = Asp.Tree.FindNode("\Data\Blocks\B35\Output\B_LTEMP\1").Value
bottomTemp =
Asp.Tree.FindNode("\Data\Streams\P3\Output\TEMP_OUT\MIXED").Value
End Sub

```


The results obtained for column T-401 show the variables for the calculation in Table 22 and the cost obtained in Table 23.

Table 22 Variables extracted from ASPEN PLUS.

N° Stage	Feed stage	Reflux	Diameter	Height	Heat Duty	Cold Duty
31	16	27.2	11.9	18.9	3.41E+02	3.41E+02
32	17	12.0	7.4	19.5	1.58E+02	1.58E+02
33	18	8.14	6.0	20.1	1.11E+02	1.11E+02
35	18	5.23	4.8	21.3	7.55E+01	7.55E+01
36	19	4.55	4.4	21.9	6.73E+01	6.73E+01
37	20	4.08	4.2	22.6	6.15E+01	6.15E+01
38	20	3.72	4.0	23.2	5.72E+01	5.72E+01
39	21	3.44	3.9	23.8	5.38E+01	5.38E+01
40	21	3.24	3.8	24.4	5.13E+01	5.13E+01
42	23	2.90	3.6	25.6	4.72E+01	4.72E+01
43	23	2.78	3.6	26.2	4.58E+01	4.58E+01
45	24	2.60	3.5	27.4	4.36E+01	4.36E+01
46	24	2.54	3.4	28.0	4.29E+01	4.29E+01
47	25	2.46	3.4	28.7	4.19E+01	4.19E+01
49	26	2.35	3.3	29.9	4.06E+01	4.06E+01
52	28	2.22	3.2	31.7	3.90E+01	3.90E+01
55	29	2.15	3.2	33.5	3.81E+01	3.81E+01
57	31	2.07	3.2	34.7	3.72E+01	3.72E+01
60	32	2.03	3.1	36.6	3.67E+01	3.67E+01
62	33	2.00	3.1	37.8	3.63E+01	3.63E+01
65	35	1.94	3.1	39.6	3.57E+01	3.57E+01
67	36	1.92	3.1	40.8	3.54E+01	3.54E+01
70	38	1.88	3.0	42.7	3.49E+01	3.49E+01
75	41	1.83	3.0	45.7	3.43E+01	3.43E+01
85	46	1.78	3.0	51.8	3.37E+01	3.37E+01
90	49	1.75	3.0	54.9	3.34E+01	3.34E+01
92	50	1.74	3.0	56.1	3.33E+01	3.33E+01
94	51	1.74	3.0	57.3	3.32E+01	3.32E+01
95	52	1.73	3.0	57.9	3.31E+01	3.31E+01
97	53	1.73	2.9	59.1	3.30E+01	3.30E+01
100	53	1.73	2.9	61.0	3.30E+01	3.30E+01

Table 23 Cost of the column detailed

N° Stage	Feed stage	Column Cost	Reboiler Cost	Condenser Cost	Utility Cost	Total Cost
31	16	2.62E+06	6.35E+03	3.93E+03	4.32E+03	2.63E+06
32	17	1.61E+06	3.84E+03	2.38E+03	1.99E+03	1.61E+06
33	18	1.31E+06	3.05E+03	1.90E+03	1.40E+03	1.32E+06
35	18	1.08E+06	2.38E+03	1.49E+03	9.55E+02	1.09E+06
36	19	1.03E+06	2.21E+03	1.38E+03	8.51E+02	1.04E+06
37	20	9.97E+05	2.08E+03	1.31E+03	7.78E+02	1.00E+06
38	20	9.74E+05	1.99E+03	1.25E+03	7.23E+02	9.78E+05
39	21	9.57E+05	1.91E+03	1.20E+03	6.81E+02	9.61E+05
40	21	9.48E+05	1.85E+03	1.17E+03	6.49E+02	9.52E+05
42	23	9.36E+05	1.75E+03	1.11E+03	5.97E+02	9.39E+05
43	23	9.36E+05	1.72E+03	1.09E+03	5.80E+02	9.40E+05
45	24	9.40E+05	1.67E+03	1.06E+03	5.51E+02	9.44E+05
46	24	9.48E+05	1.65E+03	1.05E+03	5.43E+02	9.51E+05
47	25	9.50E+05	1.62E+03	1.04E+03	5.30E+02	9.53E+05
49	26	9.64E+05	1.59E+03	1.02E+03	5.14E+02	9.67E+05
52	28	9.87E+05	1.55E+03	1.00E+03	4.93E+02	9.90E+05
55	29	1.02E+06	1.53E+03	9.92E+02	4.83E+02	1.02E+06
57	31	1.03E+06	1.50E+03	9.80E+02	4.71E+02	1.04E+06
60	32	1.07E+06	1.49E+03	9.77E+02	4.64E+02	1.07E+06
62	33	1.09E+06	1.48E+03	9.75E+02	4.59E+02	1.09E+06
65	35	1.12E+06	1.46E+03	9.69E+02	4.51E+02	1.12E+06
67	36	1.14E+06	1.45E+03	9.68E+02	4.48E+02	1.14E+06
70	38	1.17E+06	1.44E+03	9.65E+02	4.42E+02	1.18E+06
75	41	1.23E+06	1.43E+03	9.65E+02	4.35E+02	1.23E+06
85	46	1.34E+06	1.41E+03	9.71E+02	4.26E+02	1.34E+06
90	49	1.40E+06	1.40E+03	9.75E+02	4.22E+02	1.40E+06
92	50	1.42E+06	1.40E+03	9.76E+02	4.21E+02	1.42E+06
94	51	1.44E+06	1.40E+03	9.79E+02	4.20E+02	1.44E+06
95	52	1.45E+06	1.39E+03	9.79E+02	4.19E+02	1.45E+06
97	53	1.47E+06	1.39E+03	9.82E+02	4.18E+02	1.48E+06
100	53	1.51E+06	1.39E+03	9.87E+02	4.18E+02	1.51E+06

APPENDIX 9: TABLE FOR ECONOMIC EVALUATION

To obtain the equipment price from this method, the constants a and b, the equipment capacity (S) and the exponent n must be defined. These values are shown in Table 24.

Table 24. Correlations for the calculation of the equipment price.

Equipment	Description	Smín	Smáx	a	b	n
Compresor	Energy kW	75	30000	580000	20,000	0.6
Column distillation	Weight kg	160	250000	11600	34	0.85
Heat Exchanger U type	Area, m ²	10	1000	28000	54	1.2
Furnace	Energy, MW	0.2	60	80000	109000	0.8
Buffer	Weight, kg	160	250000	11600	34	0.85
Centrifugal pump	Flow l/s	0.2	126	8000	240	0.9
Reactor	Volumen m ³	0.5	100	61500	32,500	0.8
Tank	Capacity m ³	100	10000	113000	3,250	0.65
Column Tray	Diameter,m	0.5	5	130	440	1.8
Kettle	Area m ²	10	500	29000	400	0.9
Separator tank	Weight kg	160	250000	11600	34	0.85
Air cooling	Area m ²	10	500	29000	400	0.9

Table 26 shows the calculation of all equipment, with respective capacities (as specified in the table above), their price in 2010, their updated price in 2022, the installation factor, the material factor and their final cost.

In addition to the equipment, the trays that make up each column must be taken into account. The Table 25 shows the results. Carbon steel plates are considered, so the factor of 1.

Table 25 Price of the trays.

Trays	Column	Unit	S	a	b	n	Price 2010	Price 2022	Total Cost
22	T-901	Diameter (m)	4.75	130	440	1.8	7399 €	8216 €	160863 €
6	T-1101	Diameter (m)	1.6	130	440	1.8	1155 €	1283 €	6850 €
29	T-1201	Diameter (m)	2.5	130	440	1.8	2420 €	2686 €	69337 €
22	T-1301	Diameter (m)	3.03	130	440	1.8	3366 €	3738 €	73183 €

Table 25 Price of the equipment of the new section.

Quantity	Equipment	Unit	S	a	b	n	Price 2010	Price 2022	installation factor	Material factor	Total Cost
1	E-821	m2	35	28000	54	1.2	31848 €	35362 €	3.50	1.00	110152 €
1	E-822	m2	65	29000	400	0.9	46127 €	51215 €	3.50	1.00	159536 €
1	E-941	m2	200	29000	400	0.9	76096 €	84491 €	3.50	1.00	263189 €
20	E-1001	m2	162	29000	400	0.9	67960 €	75457 €	3.50	1.30	6111289 €
1	E-1121	m2	50	29000	400	0.9	42525 €	47216 €	3.50	1.00	147078 €
1	E-1221	m2	75	29000	400	0.9	48481 €	53829 €	3.50	1.00	167678 €
1	E-1321	m2	125	29000	400	0.9	59852 €	66454 €	3.50	1.00	207005 €
1	C-1005	kW	15	580000	20000	0.6	681551 €	756735 €	3.50	1.30	3064399 €
2	P-841	l/s	13.21	8000	240	0.9	10449 €	11602 €	2.00	1.00	41303 €
2	P-842	l/s	55	8000	240	0.9	16842 €	18700 €	4.00	1.00	133141 €
2	P-941	l/s	35	8000	240	0.9	13887 €	15419 €	4.00	1.00	109780 €
2	P-942	l/s	29	8000	240	0.9	12970 €	14401 €	4.00	1.00	102535 €
2	P-1241	l/s	27	8000	240	0.9	12661 €	14057 €	4.00	1.00	100087 €
2	P-1242	l/s	5	8000	240	0.9	9022 €	10017 €	4.00	1.00	71320 €
2	P-1341	l/s	22	8000	240	0.9	11876 €	13186 €	4.00	1.00	93885 €
2	P-1342	l/s	20	8000	240	0.9	11557 €	12832 €	4.00	1.00	91367 €
3	Tank	m3	800	113000	3250	0.65	363549 €	403653 €	4.00	1.00	4311010 €
3	Tank	m3	1000	113000	3250	0.65	402657 €	447075 €	4.00	1.00	4774759 €
1	Tank	m3	25000	113000	3250	0.65	2460169 €	2731558 €	4.00	1.00	9724346 €
1	T-801	kg	8500	11600	34	0.85	85985 €	95470 €	4.00	1.00	339874 €
1	T-802	kg	8500	11600	34	0.85	85985 €	95470 €	4.00	1.00	339874 €
1	T-901	kg	15000	11600	34	0.85	132147 €	146725 €	4.00	1.00	522339 €
1	T-1101	kg	2500	11600	34	0.85	37886 €	42066 €	4.00	1.00	149753 €
1	T-1201	kg	10500	11600	34	0.85	100620 €	111720 €	4.00	1.00	397724 €

1 T-1301	kg	9250	11600	34	0.85	91528 €	101625 €	4.00	1.00	361784 €
1 D-1004	kg	1400	11600	34	0.85	27658 €	30709 €	4.00	1.30	142121 €
1 R-1001	m2	25	61500	32500	0.8	488311 €	542178 €	4.00	1.30	2509199 €
1 AE-931	m2	250	29000	400	0.9	86571 €	96121 €	3.50	1.00	299418 €
1 AE-1131	m2	65	29000	400	0.9	46127 €	51215 €	3.50	1.00	159536 €
1 AE-1231	m2	73	29000	400	0.9	48013 €	53309 €	3.50	1.00	166059 €
1 AE-1331	m2	85	29000	400	0.9	50804 €	56408 €	3.50	1.00	175712 €
1 AE-1003	m2	100	29000	400	0.9	54238 €	60221 €	3.50	1.30	243867 €
1 H-501	MW	35	80000	109000	0.8	1953617 €	2169127 €	2.00	1.30	5019360 €
1 D-931	kg	12500	10200	31	0.85	104332 €	115841 €	4.00	1.00	412393 €
1 D-1131	kg	500	10200	31	0.85	16302 €	18101 €	4.00	1.00	64438 €
1 D-1231	kg	500	10200	31	0.85	16302 €	18101 €	4.00	1.00	64438 €
1 D-1331	kg	12087	10200	31	0.85	101681 €	112898 €	4.00	1.00	401917 €