



Treball Final de Grau

Design of a plant for bioethanol production from sugarcane.

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June 2021



UNIVERSITAT DE
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If you can't explain it simply, you don't understand it well enough.

Albert Einstein

REPORT

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SUMMARY

The following report presents of the preliminary design of a bioethanol plant from sugarcane. To design the plant, it is necessary to choose its location, the type of sugarcane and the optimal conditions for its plantation. The plant is divided into three stages: food conditioning, fermentation and ethanol purification. Sugarcane is made up of sucrose, water, fiber, and impurities. Depending on the type of cane used and the environmental conditions of the plantation, the percentage of sucrose will be modified. In this case, it is interesting that this amount be as high as possible since it will be the one that is later fermented and provides us with the desired compound.

The food conditioning consists firstly in the milling of the cane to obtain the water and the sucrose and discard the fiber. Next, it goes on to clarification where the pH is adjusted with SO_2 to optimize the process and it is alkalinized to adjust the Baumé degrees using milk of lime. Finally, the juice is heated and fermented. In this stage, sucrose is first transformed into fructose and glucose by adding an enzyme and then, these are fermented in ethanol by adding the yeast *Saccharomyces Cerevisiae*.

Finally, we proceed to the ethanol purification, for this first a Flash separator is necessary that is responsible for the separation of the CO_2 generated in the fermenter. Next, it is passed to the first distillation column in which a mixture of ethanol and water close to the composition of the azeotrope is obtained at the top of the column and finally, it is passed to the second column in which an extracting agent, MTBE, is added. in this case, to purify the ethanol to a composition of 99.7%.

Keywords: Bioethanol, sugarcane, food conditioning, fermentation, ethanol purification, sucrose, *Saccharomyces Cerevisiae*, MTBE.

RESUM

La següent memòria presenta el disseny preliminar d'una planta de producció de bioetanol a partir de canya de sucre. Per a poder dissenyar la planta és necessari escollir la seva ubicació, el tipus de canya a utilitzar i les condicions òptimes per a la seva plantació. La planta es divideix en tres etapes: condicionament de l'aliment, fermentació i purificació de l'etanol. La canya de sucre està composta per sacarosa, aigua, fibra i impureses. Depenent del tipus de canya que s'utilitzi i les condicions ambientals de la seva plantació el percentatge de sacarosa es veurà influenciat. En aquest cas, interessa que aquesta quantitat sigui el més gran possible ja que, aquest es el que es fermenta i proporciona el compost desitjat.

El condicionament de l'aliment consisteix primerament en la mòlta de la canya per tal d'obtenir l'aigua i la sacarosa i rebutjar la fibra. Seguidament, es passa a la clarificació on s'ajusta el pH amb SO₂ per tal d'optimitzar el procés i s'alcalinitza per tal d'ajustar els graus Baumé mitjançant lletada de calç. Finalment, s'escalfa i es passa a la fermentació d'aquest. En aquesta etapa primerament es transforma la sacarosa en fructosa i glucosa mitjançant l'adició d'un enzim i finalment, estes es fermenten en etanol mitjançant l'adició del llevat *Saccharomyces Cerevisiae*.

Finalment, es passa a la purificació de l'etanol. Per fer-se primerament es necessari un separador Flash que s'encarrega de la separació del CO₂ generat al fermentador. Seguidament, es passa a una primera columna de destil·lació on s'obté per cap de columna una mescla d'etanol i aigua a prop de la composició del seu azeòtrop i finalment, es passa a una segona columna on s'afegeix un agent extractor, MTBE en aquest cas, per tal de purificar l'etanol fins a una composició del 99.7%.

Paraules clau: Bioetanol, canya de sucre, condicionament de l'aliment, fermentació, purificació del etanol, sacarosa, *Saccharomyces Cerevisiae*, MTBE.

1. INTRODUCTION

1.1. HISTORY

30 years ago, when a liter of ethanol was worth three times as much as a liter of gasoline, very few countries would have considered investing in it as fuel. But Brazil did so thanks to its favorable conditions and now produces the cheapest ethanol in the world.

In 1973 the industry progressed thanks to an international oil crisis that doubled spending on imports and the Brazilian government was forced to consider alternative sources of energy. He invested to increase agricultural production, modernize and expand distilleries, and establish new production plants. Causing that in the following 15 years ethanol production increased enormously from 0.6 billion liters in 1975 to 11 billion in 1990^[1].

Waste became a problem at that time. Stillage, a corrosive liquid byproduct of ethanol distillation, was dumped into rivers, causing environmental damage. But then stillage was found to be good fertilizer, and in the 1980s Braunbeck and a team from the Sugarcane Technology Center developed a transportation system that involved a combination of trucks, pipes, and pipelines to carry stillage from the distilleries to the fields ^[1].

Researchers from the General Command for Space Technology and other institutes also found ways to use leftover sugarcane fiber, known as bagasse, to produce energy using existing burning methods to drive steam turbines and generate electricity. They developed higher pressure boilers to produce more energy, allowing many ethanol plants to become self-contained in terms of energy. This contributed significantly to keeping ethanol production at low costs.

Nowadays, Brazil is the second-largest ethanol producer in the world with a production of 20 billion liters after the United States. 80% of this is for the domestic market and the fuel used in 45% of Brazilian vehicles is ethanol. All of this is possible because Bosch engineers developed cars that allow flexible fuel use, running on gasoline, ethanol, or a mixture of both.

Brazil has many challenges to face to remain at the forefront of the ethanol market. Producing ethanol from sugarcane bagasse will be a step in this direction. This will make it possible to obtain ethanol without wasting the cane, but there are currently doubts about the economic viability of the process [1].

1.2. IMPORTANCE OF BIOETHANOL

Ethanol is a colorless liquid compound known to be the main component of alcoholic beverages, but this is not its only use. This can be used as a fuel for automobiles by itself or mixed with gasoline in variable quantities to reduce the consumption of petroleum derivatives. The most common mixtures are E10 and E85, containing 10% and 85% ethanol, respectively. It can also be used to oxygenate standard gasoline replacing tert-butyl ether, as it causes considerable soil and groundwater contamination [2].

Ethanol from crop fields is emerging as a potentially sustainable energy resource that can offer long-term environmental and economic benefits over fossil fuels [2].

Bioethanol can be used to produce biofuels of high energy power with characteristics very similar to those of gasoline, which lead to a significant reduction in polluting emissions or be mixed in concentrations of 5% (E5) or 10% (E10) without producing any change in the motors currently working [3].

Bioethanol is obtained from the fermentation of agricultural products such as corn, wheat, barley, beets, sugar cane, sorghum, among others [3].

On a commercial scale, Brazil and the US have successfully and massively implemented ethanol as fuel and are the main producers of bioethanol, together accounting for 80% of world production. Despite this, neither the United States nor Europe would currently be able to be self-sufficient using this type of fuel due to a lack of land to grow the raw material [4].

Brazil is the main producer of bioethanol from sugar cane, it uses modern equipment achieving a very competitive ethanol price and a high energy balance. The United States generates bioethanol from corn for the most part. Brazil generates a productivity per planted hectare of 6 800 – 8 000 liters of ethanol per hectare, as opposed to the 3 800–4 000 that the United States generates. The energy balance is also much higher for Brazil with a ratio of the

energy obtained to the energy used for its production of 8.3 to 10.2 times, as opposed to 1.3 - 1.6 times for the United States [4].

1.3. CHARACTERISTICS OF BIOETHANOL

Ethanol is a chemical compound that under normal conditions of temperature and pressure is a colorless and flammable liquid with a boiling point of 78.4 °C. In *Table 1* we can see its physical, chemical, and thermochemical characteristics [4].

Table 1. Ethanol Properties [4]

Appearance	Color Less
Density [kg/m³]	789
Molecular Mass [g/mol]	46.07
Melting Point [°C]	-114
Boiling Point [°C]	78
Critical Temperature [°C]	241
Critical Pressure [atm]	63
Solubility	Miscible
Enthalpy Vaporization [kJ/mol]	-235.3
Liquid Enthalpy [kJ/mol]	-277.6

Another characteristic of ethanol in the presence of an ethanol-water azeotrope. This makes it impossible to separate them at a composition greater than 95.63% in ethanol without the use of an extracting agent, using ionic liquids, or heterogeneous extraction, among others [5].

1.4. GENERAL DESCRIPTION OF THE PROCESS

The production of bioethanol from sugar cane can be defined in three stages: food conditioning, fermentation, and ethanol purification.

Sugarcane is mainly made up of 70-75% water, 10-15% sucrose, 10-15% fiber, and approximately 3% impurities, these would be other simple sugars such as glucose or fructose, oligosaccharides, polysaccharides, colorants such as phenols or flavonoids, amino acids,

proteins, organic or inorganic acids such as salts of potassium, phosphate, calcium, magnesium, iron ... These values vary depending on the type of cane or its maturation [6].

1.4.1. Food Conditioning

The reception of the cane is the stage of the sugar and ethanol production process. Upon arrival at the mill, the cane is weighed and analyzed in the laboratory to determine the amount of sucrose it contains.

Later, the sugarcane will be washed on the feeder tables to remove impurities and foreign matter from the crop. During the preparation stage, the cane will be chopped, shredded, and leveled to be sent to the mills.

1.4.1.1. Milling

Milling is the stage in which the juice is extracted through the use of mills as represented in *Figure 1*.

The basic functions of milling are as follows [7]:

- Mill a quantity of cane according to its capacity.
- Extract the maximum of the juice content and take out that the cane brings.
- Deliver bagasse in the conditions for the boilers.

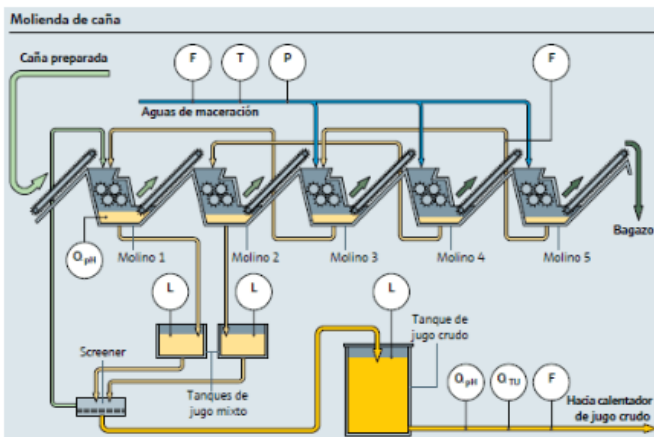


Figure 1. Cane milling [8]

The juice extracted in the first phase of milling is known as rich or primary juice. The second phase is known as poor or secondary juice since it went through an imbibition process in the last phase, where water was added. The mixture of the primary and secondary juices is called mixed juice and this is pumped into a strainer to remove the bagasse.

At this stage, the fiber contained in the sugar cane and a small part of the sucrose and water are discarded, forming the bagasse. The bagasse is used as fuel for the boilers. Poor mill operation creates situations that are difficult to control in other areas of the plant. For example, if humidity levels of 50% are not reached in the bagasse, the steam generation will be directly affected. If you do not have strict control of the imbibition, with the proper flow and temperature, it will affect the extraction of sucrose and, therefore, the work of the areas of juice purification and evaporation.

At the entrance of the last mill, soaking water is added to dilute the juice and extract the sucrose contained in the fibrous material. The juice content that results from each extraction is sent to the previous mill and so on until the second. The juice content extracted by the first and second mills is sent to the processing stage.

1.4.1.2. Filtration

The juice extracted during milling contains a lot of suspended bagasse, generally known as bagasse. To remove it, the juices are first passed through perforated filters with 1 mm diameter holes. The most common form consists of fixed horizontal filters. As it passes through the filter, the juice is deposited in a tank and the bagasse that has been separated is collected using a scraper conductor that takes it back to the mills. The filtered juice is pumped to the clarifier ^[9].

1.4.1.3. Clarification

- Sulfidation

In this stage, an absorption reaction of SO₂ takes place with the juice until a pH of between 4 and 4.6 is achieved.

The juice enters through the upper part of the tower and falls by gravity into a dosing tank where its pH will be adjusted; while in the opposite direction (from bottom to top) sulfur gases pass through which are captured by the juice on its way down the tower.

Sulfur gases (SO₂) are produced by the combustion of solid sulfur (granules) which are introduced to the towers through an induced draft carried out by fans located on an upper floor, forcing the gases to enter through the lower part of the towers and on their way, they are captured by the juices that descend through them ^[9].

- Alkalization

As the sulfidation operation entails a decrease in the pH of the juice and at its values, the inversion of sucrose is favored, therefore, it is necessary to neutralize the juice, which is achieved by adding milk of lime (lime dissolved in water and at a concentration of 6 to 10 °Bé (degrees Baumé)). Also, alkalization (defecation) occurs, calcium ions react with most of the impurities that the juice carries, forming solids that precipitate easily separating them ^[9].

- Heating

The juice already sulfated and alkalized, through the use of pumps, is passed through a series of heaters where the temperature is raised first to 70-75 °C and then to 102-105 °C for the purpose of accelerating the reaction for defecation, protecting the juice making pasteurization, denaturing the proteins and eliminating the dissolved air and/or the bagasse ^[9].

- Flocculant addition

To accelerate the precipitation, flocculants (chemical helpers) are used, they are synthetic polymers which, when in contact with the juice, extend their polymer chains creating a kind of cobweb which, as it rises by gravity, captures regularly cationic impurities ^[9].

1.4.2. Fermentation

The fermentation process is the transformation of an organic substance into another desired one, this process is carried out thanks to the addition of a ferment.

In this case, we start from sucrose, a molecule made up of glucose and fructose as seen in *Figure 2*. When hydrolyzed, the bond breaks, and a glucose molecule and a fructose molecule are obtained.

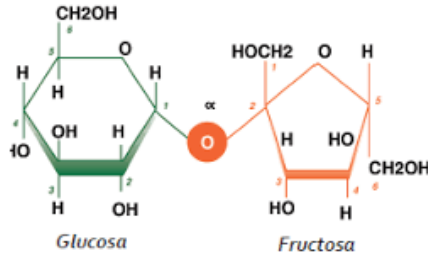
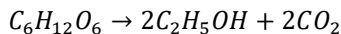


Figure 2. Saccharose molecule ^[10]

Its two molecules are those that are transformed into alcohol and CO₂ thanks to fermentation with the corresponding yeast. For the bioconversion of hexose in ethanol, the most commonly used microorganism is *Saccharomyces cerevisiae*. It has a high resistance to ethanol, consumes significant amounts of the substrate under adverse conditions, and shows high resistance to inhibitors present in the medium. Fermentation follows the following reaction ^[11]:



Saccharomyces Cerevisiae yeast works optimally at a temperature between 28 and 35 °C, the optimum being 32 °C. Yeast is affected at high concentrations of alcohol, it begins to influence when it exceeds 3% and after 10% its growth is completely paralyzed, therefore it is important not to exceed this concentration. The pH is also an important factor in the fermentation process since it controls the contamination by microorganisms foreign to the process and influences the growth of the yeast, therefore, the production of ethanol. During the process, the yeast takes nitrogen from organic amino acids, thus losing its amphoteric character and becoming acidic. This causes a reduction in the pH of the medium and the lower the pH the more likely contamination is and the fermentation slows down. The pH range for *Cerevisiae* is between 4.4 and 5.5, being optimum for growth 4.5 ^[11].

The quantities of air required for the production of yeast vary between 0.017 and 0.033 m³ of air per gram of yeast. At the beginning of the fermentation, the aeration power should not be very intense since in these initial moments the alcohol concentration is small and the medium becomes susceptible to being infected by other microorganisms. By increasing the oxygen concentration, the conditions for biomass growth are improved, but this causes the substrate invested in ethanol production to decrease, thereby reducing the efficiency of ethanol production ^[11].

Saccharomyces Cerevisiae withstands high concentrations of sugars, 22% v/v and allows an approximate conversion of 85% after 32 hours and 90% after 75 hours in the production of ethanol. Under aerobic conditions, the maintenance energy is 0.022 grams of cells per gram of substrate and hour [11].

Once the ethanol has been produced, it is centrifuged and decanted in order to recover all the yeast and obtain only the water, ethanol, carbon dioxide and the unreacted remains of sucrose, fructose and glucose.

1.4.3. Purification

The last step consists of purifying the ethanol to achieve a purity of between 99.5% and 99.9% in ethanol. This separation is not so simple since the water-ethanol mixture presents an azeotrope in 95.6% ethanol and this purity is not sufficient for its use as fuel. Various separation options are using various extracting agents, but in this case, it will be carried out by heterogeneous catalysis using MTBE since the use of extracting agents such as cyclohexane or benzene, one of the most common, are too polluting, another option is physical adsorption through molecular sieves, but this generates a higher cost [12].

To use the minimum amount of extracting agent, first, the composition of the desired stream must be brought as close as possible to the azeotrope and then the minimum MTBE necessary for the complete extraction of ethanol is introduced and pure ethanol is obtained, knowing that the solubility of water in MTBE it is 1.5% by weight [13].

2. OBJECTIVES

The main objective of this project is the design of a bioethanol production plant.

To achieve this objective, it is necessary to choose the optimal sugarcane variety for the process.

Next, it is necessary to select the appropriate process and the optimal conditions to carry it out. To do this, it must be taken into account that the process has to be as cheap as possible.

The place in which to build the plant should be selected so that the conditions are ideal for the growth of the cane.

Also, the main equipment involved in the process is dimensioned using empirical equations and using the *Aspen Plus V11* ® program.

3. PLANT LOCATION

Sugarcane does not withstand temperatures below 0 °C and needs a minimum of 14 to 16 °C to be able to grow, being the optimum growth of 30 °C with a high relative humidity and a good supply of water. Best suited to light soils. For this reason, Brazil is a good country in which to plant sugar cane since, the warmest month its highest temperature is about 30.4 °C and the coldest its lowest temperature is 14.6 °C, therefore, the growth of the plant will never be stopped even though its growth is not optimal all year round. Relative humidity varies between 87% in the wettest month and 45% in the least humid month, therefore, humidity is generally also at high values ^[14].

The northern part of the country is the one with a warmer climate and higher humidity since it is located next to the Amazon River. Therefore, this will be the area where you will find a better quality of the cane and therefore, the best area to build the plant ^[15].

Alagoas may be the ideal region to build the production plant since it is located in the northern part of the country as seen in *Figure 3* and cultivates 5.26% of the country's sugar cane ^[16].

This city can also be a good place to install the plant due to its proximity to the sea and the ease that this entails for the export of the bioethanol generated or the arrival of raw materials necessary to produce this.



Figure 3. location of Alagoas in Brazil ^[17]

4. SELECTION OF THE VARIETY OF THE SUGAR CANE

There are different varieties of sugar cane where, depending on the needs, the use of one or the other is optimal. To produce bioethanol, the selected varieties must have a high number of stems and respond affirmatively to the use of fertilizer, in addition to being able to accept the use of supplementary fertilizer applications to increase their growth. They must also respond to chemical ripeners such as POLARIS and ETHEL so that vegetative growth can be reduced very quickly, and the sugars deposited on the stems are not used as energy for growth. The selected varieties must have complete foliage of green leaves, six weeks before the harvests, this is the period in which the chemical ripeners are injected ^[18].

The rate of supplemental fertilizer application ranges from 100 to 200 pounds of muriate of potassium per hectare of application. Strong phosphate fertilizers are applied to the seed at sowing to accelerate root growth and stem development.

In the ripening process, sucrose accumulates in the stem and for this, a relative decrease in growth speed is required. The goal is to get the maximum amount of sucrose in the stem.

The ideal cane to produce alcohol must be at its optimum point of maturity, be strawberry, with the time between cutting and milling of a maximum of 24 to 48 hours and free of mineral and vegetable impurities. Times longer than this can cause losses greater than 5% of sugar ^[18].

A study has been launched for the development of a variety of genetically modified sugarcane thanks to the Canaviera Technology Center (CTC) together with the Interuniversity Network for the Development of the Sucrenergic Sector (Ridesa) and the Agronomic Institute of Campinas (IAC). In 2018, it was accepted by the body responsible for the analysis of the biosafety evaluation of genetically modified organisms (GMOs) to commercialize the first transgenic sugarcane in Brazil ^[18].

This new variety, baptized with the name CTC 20 Bt, is resistant to the *Diatraea Saccharalis* moth, the main pest of Brazilian reed beds. Varieties have been produced from this genetic modification, the EC-05 variety being the most efficient as can be seen in *Figure 4* ^[19].

Variedad	Producción de caña (TCH)	Rendimiento de azúcar (KATC)	Sacos [§] /ha
EC-05	74.0	113.4	167
EC-06	69.5	109.3	154
ECU-01	74.5	108.4	165
CC85-92	76.5	112.2	172
Ragnar	52.8	112.8	120

TCH=Toneladas de Caña/ha. KATC=Kilogramos de Azúcar/tonelada de Caña. § = Saco de 50 kg de azúcar.

Figure 4. Sugarcane varieties ^[19]

Together, a study has been done looking at the degree of reaction to the following cane diseases (Figure 5).

ENFERMEDAD	EC-05
Carbón , <i>Sporisorium scitamineum</i> (Syd.) M. Piepenbr., M. Stoll & Oberw. 2002	Altamente resistente
Mosaico , <i>Sugarcane mosaic virus SCMV-Potyvirus</i>	Altamente resistente
Roya café , <i>Puccinia melanocephala</i> H. Sydow. & P. Sydow	Intermedia [§]
Roya naranja , <i>Puccinia kuehnii</i> (W. Krüger) E.J. Butler	Resistente ^{§§}
Raquitismo , <i>Leifsonia xyli</i> subsp <i>xyli</i> Davis et al.	Susceptible
Hoja amarilla , <i>Sugarcane yellow leaf virus, SCYLV</i>	Tolerante

Figure 5. EC-05 reaction to various diseases ^[19]

It can be concluded that the result has been quite favorable, and that this variety could be the optimal one for rapid and greater growth of the cane.

5. PROCESS SELECTION

The first idea of the design of the process is given by the bibliography ^[20] but this process is slightly modified by the age of the process and the use of an excessively harmful extracting agent that is no longer used today.

Two options are proposed to guarantee the lowest possible cost of the process in the purification stage.

Once the fermentation stage is finished and the yeast is separated, ethanol and CO₂ are obtained along with the rest of the unreacted compounds. All components are heavier than ethanol and water except carbon dioxide. Therefore, using a distillation column directly will produce ethanol, water, and carbon dioxide per head of the column. To avoid this, one option is to place a flash-type separator before the distillation column in which the CO₂ will be eliminated through the head and the subtraction of compounds will be obtained through the foot (*Figure 6*).

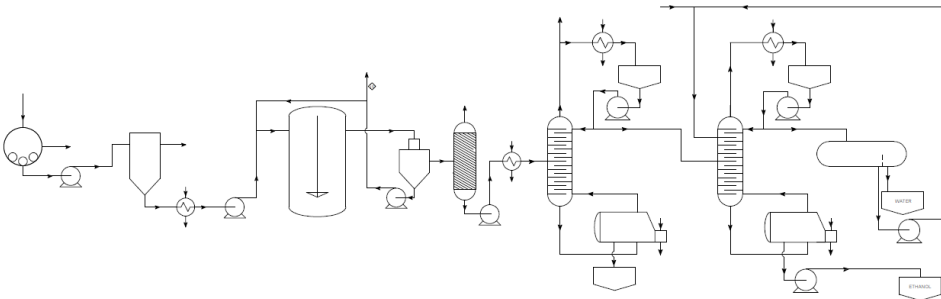


Figure 6. Process that operates with flash separator

Another option would be to introduce the mixture directly into the distillation column and incorporate a partial condenser to separate the carbon dioxide later. This will increase the cost of the column since it will have to be larger when introducing a gas (*Figure 7*).

As indicated in the table, the most economical option, therefore, the one that will be designed is the use of a Flash separator to eliminate the CO₂ before the first distillation column.

6. PFD

The nomenclature is made up of a letter and three numbers. The first letter of the nomenclature indicates the type of equipment that is being used.

M: mill

B: pump

C: clarifier

I: exchanger

R: reactor

S: separator

C: column

T: tank

The first number indicates the area of the process you are in.

Being:

1. Food conditioning
2. Reactor
3. Purification

The second and third numbers indicate the subgroup of each.

The material balances can be seen in *Appendix I*.

7. DESIGN AND SPECIFICATIONS EQUIPMENT

The sugar cane used for the design of this process is made up of 12% sucrose, 71% water, 14% fiber, and approximately 3% impurities. This composition can vary depending on the time of year and the conditions in which the plantation is at that time.

A calculation base of 108 200 kg/h of sugar cane has been chosen for the design of the plant.

During the milling process, the fiber is removed from the process and during clarification certain impurities and a small part of the sucrose and water constituents in the cane are discarded.

A flow rate of 82 000 kg/h corresponds to the design of the equipment and the one that reaches the fermenter, the first stage designed in this process.

7.1. FERMENTER (R-211)

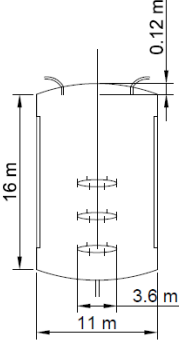
For the process, a Batch-type operating system has been chosen in which fermentation and glucose hydrolysis will take place in a single stage.

First, the saccharification of the dextrins is carried out thanks to the action of the glucoamylase enzyme which is continuously fed to the reactor. This enzyme is responsible for breaking down the sucrose molecule to generate a glucose molecule and a fructose molecule. The amylase extracted from barley will be used since it operates at a temperature of between 30-39 °C and a pH of between 4.7 and 5.8, therefore, the operating conditions are defined as optimal for fermentation. An amount of 0.5% weight/volume is necessary, therefore, 60 kg/h of the enzyme [21].

Subsequently, the fermentation will be carried out at 32 °C and a pH of 5 for an operation time of 14 hours [20] and with *Saccharomyces Cerevisiae* as the yeast used. With a conversion of 90%, an ethanol concentration of 7% by mass is obtained [21].

Once the operating conditions have been decided, the reactor design is carried out, the calculation method chosen for each equipment specification is included in *Appendix II* and these are represented in *Table 4*. The material is chosen following *Appendix VIII*.

Table 4. R-211 Spec Sheet

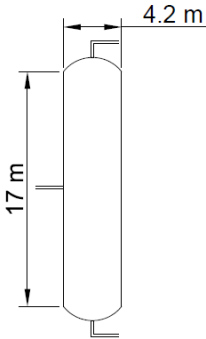
Design Parameter	Value
Tank volume [m ³]	1 470
Temperature [°C]	32
pH	5
Operation time [h]	14
Tank diameter [m]	11
Tank height [m]	16
Dome volume [m ³]	5.5
Dome height [m]	0.12
Real volume [m ³]	1 500
Agitator	Rushton turbine
Number of agitator blades	6
Agitator diameter [m]	3.6
Turbine blade height [m]	0.72
Turbine blade width [m]	0.9
Agitator useful height [m]	7.2
Number of baffles	4
Baffle spacing [°]	90
Motor power [kW]	3 000 000
Material	AISI 304
Sketch	

7.2. FLASH (S-311)

A Flash separator is designed to eliminate the carbon dioxide formed in the fermenter. To optimize the equipment, an attempt is made to carry out the design by previously placing a pump and an exchanger to the separator to heat the fluid. This is impossible as the pump generates cavitation problems for any offered pressure. For this reason, it is necessary to feed the separator under the conditions coming from the fermenter (32 °C and 1 bar) and generate the pressure and temperature difference by operating the Flash at 0.1 °C and 0 bar. In this way, it is possible to separate 96% of the CO₂ generated in the fermenter, being simulated with Aspen Plus V11 ®.

The equipment sizing is carried out following the heuristics indicated in *Appendix III*. The values obtained are tabulated in *Table 5*. The material is chosen following *Appendix VIII*.

Table 4. S-311 Spec Sheet

Design Parameter	Value
Temperature [°C]	0
Pressure [bar]	0.1
Feed flow [kg/h]	82 000
Area [m ²]	14
Diameter [m]	4.2
Height [m]	17
Allowed steam velocity [m/s]	0.6
Material	AISI 304
Sketch	

7.3. COLUMN (C-321/C-331)

The distillation columns have been designed using the *Aspen Plus V11*® program. It has been designed according to the RadFrac distillation column model and using the NRTL composition model since this is the one that best adjusts to the compounds involved in the process. To optimize the columns and obtain the highest performance at a lower cost, the number of plates, the feed plate, and the reflux flow has been optimized. In the C-321 column, the unreacted residues of sucrose, glucose, and fructose are fed together with the CO₂ not eliminated in the previous separator and the water and ethanol. Water and ethanol form an azeotrope at 95.6% in ethanol, the intention is to reach this point for such that in the second column with MTBE to obtain ethanol at 99.7%, but when trying to optimize the process it is observed that it is very difficult to achieve this point and a too expensive column would be necessary for this reason, a water-ethanol mixture at 80% in ethanol is obtained from the first column 80% ethanol is fed into column C-331 along with the required amount of MTBE. MTBE absorbs 0.5% by mass of water, therefore 60 192 kg/h of MTBE are required [22]. The same parameters are optimized as for the first column. *Table 6* shows the main parameters necessary for the design of C-321 and *Table 7* those of C-331. The material is chosen following *Appendix VIII*.

Table 5. C-321 Spec Sheet

Design Parameter	Value
Type of contact	Plates
Operation mode	Continuous
Reflux ratio	2.445
Pressure [bar]	1
Feed flow [kg/h]	76 197
Height [m]	6.7
Diameter [m]	2.2
Number of plates	13
Feeding plate	11
Spacing between plates [m]	0.61
Plate diameter [mm]	13
Plate thickness [mm]	51
Weir height [m]	0.051
Weir length [m]	1.6

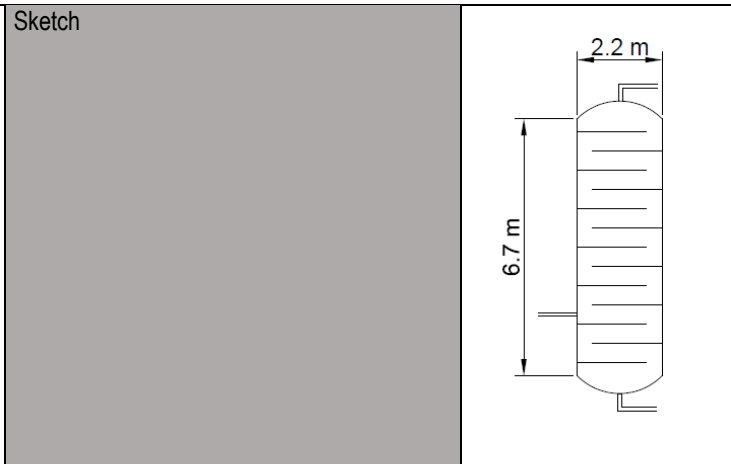
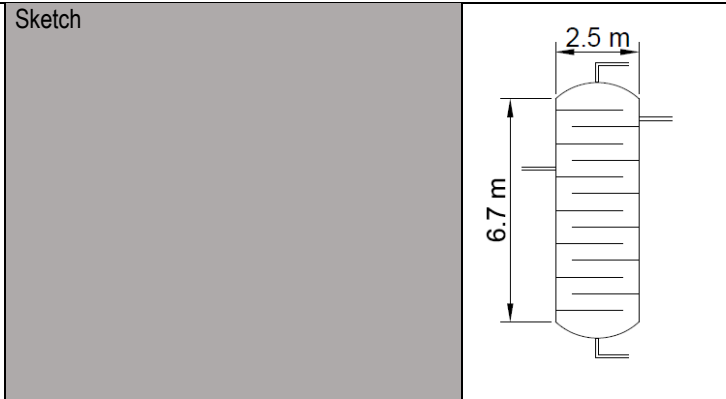


Table 6. C-331 Spec Sheet

Design Parameter	Value
Type of contact	Plates
Operation mode	Continuous
Reflux ratio	1.1
Pressure [bar]	1
Feed flow [kg/h]	61 417
Height [m]	6.7
Diameter [m]	2.5
Number of plates	13
Ethanol-water feeding plate	5
MTBE feeding plate	2
Spacing between plates [m]	0.61
Plate diameter [mm]	13
Plate thickness [mm]	51
Weir height [m]	0.051
Weir length [m]	1.8



7.4. EXCHANGERS

The process contains six heat exchangers. Shell and tube exchangers have been chosen as the flow rate is considerable. To calculate the necessary flow, it is done using the following equation.

$$Q = w \cdot Cp \cdot \Delta T$$

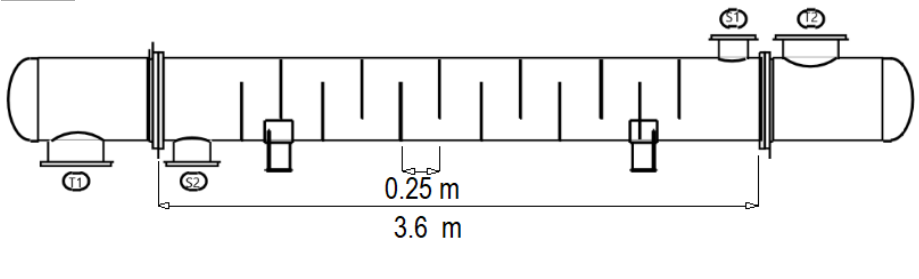
7.4.1.I-114

The first exchanger is placed to adapt the food to the operating conditions of the fermenter since it operates at 32 °C and the clarifier outlet is at 95 °C. For this, tap water is used that passes according to the theoretical calculation from 10 °C to 20 °C, this is not really due to the pressure losses obtained in the real design of *Aspen Plus V11* ®.

In *Table 8* are the specifications obtained, to design the equipment with the Aspen program it is necessary to define some previous parameters, the previously defined calculations and parameters are found in *Appendix IV*. The material is chosen following *Appendix VIII*.

Table 7 I-114 Spec Sheet

Design Parameter	Value
Type	BEM
Tube bundle type	Fixed tubular plate
Heat flow [kW]	5 740
Cold fluid inlet temperature	97
Cold fluid outlet temperature	32
Hot fluid inlet temperature	10
Hot fluid outlet temperature	15.3
Pitch [mm]	23.81
Tube pattern	30 / Triangular
Shell ID [m]	0.5
Shell OD [m]	0.51
Tube length [m]	3.6
Number of baffles	12
Baffle spacing center-center [m]	0.25
Baffle cut orientation	Horizontal
Number of tubes	323
Material	AISI 304

Sketch**7.4.2.I-313**

The second exchanger serves to heat the food before feeding to the first column since, after the Flash separator, the fluid is at 0.1 °C. To heat the fluid to a temperature of 28 °C, water vapor is used at a temperature according to the theoretical calculation of 140 °C, cooling down to a temperature of 130 °C. This is not true due to the pressure drops obtained in the real *Aspen Plus*

V11 © design. In *Table 9* are the specifications obtained, to design the equipment with the Aspen program it is necessary to define some previous parameters, the calculations and previously defined parameters are found in *Appendix IV*. The material is chosen following *Appendix VIII*.

Table 8. I-313 Spec Sheet

Design Parameter	Value
Type	BEM
Tube bundle type	Fixed tubular plate
Heat flow [kW]	2 340
Cold fluid inlet temperature	140
Cold fluid outlet temperature	130.5
Hot fluid inlet temperature	0.36
Hot fluid outlet temperature	28
Pitch [mm]	23.81
Tube pattern	30 / Triangular
Shell ID [m]	0.9
Shell OD [m]	0.91
Tube length [m]	1.8
Number of baffles	6
Baffle spacing center-center [m]	0.2
Baffle cut orientation	Horizontal
Number of tubes	1 192
Material	AISI 304
Sketch	

7.4.3.1-322

The exchanger of the first column consists of a partial condenser to condense all the fluid except the remains of carbon dioxide. For its design, running water is used that is heated from 20 to 30 °C without taking into account the pressure drops. In *Table 10* are the specifications obtained, to design the equipment with the *Aspen* program it is necessary to define some previous parameters, the calculations and previously defined parameters are in *Appendix IV*. The material is chosen following *Appendix VIII*.

Table 9. 1-322 Spec Sheet

Design Parameter	Value
Type	BEM
Tube bundle type	Fixed tubular plate
Heat flow [kW]	5 354
Cold fluid inlet temperature	10
Cold fluid outlet temperature	12.7
Hot fluid inlet temperature	45.77
Hot fluid outlet temperature	40.78
Pitch [mm]	23.81
Tube pattern	30 / Triangular
Shell ID [m]	0.5
Shell OD [m]	0.51
Tube length [m]	1.95
Number of baffles	2
Baffle spacing center-center [m]	0.6
Baffle cut orientation	Horizontal
Number of tubes	240
Material	AISI 304
Sketch	

7.4.4.I-325

The first column reboiler is designed using *Aspen Plus V11*® and the designed parameters are tabulated in *Table 11*. To heat the fluid, steam is used to 140 °C and the necessary flow is calculated to reach 130 °C theoretically. In *Appendix IV* you will find the considerations made for the design of the equipment. The material is chosen following *Appendix VIII*.

Table 11. I-325 Spec Sheet

Design Parameter	Value
Type	BKU
Tube bundle type	U
Heat flow [kW]	11 414
Cold fluid inlet temperature	98.2
Cold fluid outlet temperature	99.2
Hot fluid inlet temperature	140
Hot fluid outlet temperature	130.5
Pitch [mm]	23.81
Tube pattern	90 / Square
Shell ID [m]	2.5
Shell OD [m]	2.53
Tube length [m]	6
Number of tubes	7 160
Tube passes	8
Material	AISI 304
Sketch	

7.4.5.I-332

A total condenser is used since the remaining amounts of carbon dioxide are practically nil. To cool the fluid, tap water is used to 10 °C and the necessary flow is calculated to reach 20 °C theoretically. It is designed using *Aspen Plus V11* ® and the designed parameters are tabulated in *Table 12*. In *Appendix IV* you will find the considerations made for the design of the equipment. The material is chosen following *Appendix VIII*.

Table 12. I-332 Spec Sheet

Design Parameter	Value
Type	BEM
Tube bundle type	Fixed tubular plate
Heat flow [kW]	6 305
Cold fluid inlet temperature	10
Cold fluid outlet temperature	14.66
Hot fluid inlet temperature	44.42
Hot fluid outlet temperature	38.06
Pitch [mm]	23.81
Tube pattern	30 / Triangular
Shell ID [m]	0.675
Shell OD [m]	0.68
Tube length [m]	2.7
Number of baffles	2
Baffle spacing center-center [m]	0.59
Baffle cut orientation	Horizontal
Number of tubes	476
Material	AISI 304
Sketch	

7.4.6.I-337

The second column reboiler is designed using *Aspen Plus V11*® and the designed parameters are tabulated in *Table 13*. To heat the fluid, steam is used to 140 °C and the necessary flow is calculated to reach 130 °C theoretically. In *Appendix IV* you will find the considerations made for the design of the equipment. The material is chosen following *Appendix VIII*.

Table 13. I-337 Spec Sheet

Design Parameter	Value
Type	BKU
Tube bundle type	U
Heat flow [kW]	6 260
Cold fluid inlet temperature	77.6
Cold fluid outlet temperature	74.5
Hot fluid inlet temperature	140
Hot fluid outlet temperature	130.3
Pitch [mm]	25.4
Tube pattern	90 / Square
Shell ID [m]	1.98
Shell OD [m]	1.99
Tube length [m]	3
Number of tubes	4 500
Tube passes	2
Material	AISI 304
Sketch	

7.5. DECANTER (S-335)

A decanter is used to separate a small part of the water-MTBE that is obtained at the top of the column in the second distillation column. This amount is minimal since the amount of MTBE necessary to absorb all the water is used.

First, the type of decanter suitable for this process has been chosen. A continuous gravity decanter is used. This type of decanter is used due to the difference in density between the water and the MTBE. *Table 14* shows the calculated specifications and the procedure used for the calculation in *Appendix V*. The material is chosen following *Appendix VIII*.

Table 14. S-335 Spec Sheet

Design Parameter	Value
Temperature [°C]	44.4
Pressure [bar]	1.1
Feed flow	29 246
Inlet viscosity [cP]	0.29
Heavy phase outlet flow [kg/h]	53.1
Light phase outlet flow [kg/h]	29 133
Heavy phase density [kg/m ³]	960
Light phase density [kg/m ³]	721.6
Separation time [min]	7.2
Volume [m ³]	5.34
Length [m]	7
Diameter [m]	1.4
Head type	Torispherical
Thickness [mm]	5
Material	AISI-304
Sketch	

7.6. TANKS

There are 5 tanks during the process, their functions are defined in *Table 15*.

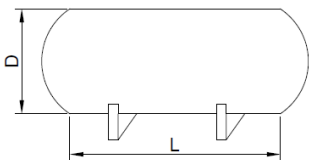
Table 15. Production process tanks

Name	Function
T-323	Buffer tank after the condenser of the first column
T-326	Storage tank reboiler outlet of the first column
T-333	Buffer tank after second column condenser
T-336	Storage tank pure water obtained from the decanter
T-339	Ethanol storage tank

In *Appendix VI* you will find the necessary calculations for the design of the specifications of each one. The material is chosen following *Appendix VIII*.

Table 16 tabulates the specifications for all tanks.

Table 16. Production process tank specifications

Design Parameter	T-323	T-326	T-333	T-336	T-339
Temperature [°C]	45.8	98.8	44.4	44.4	77.6
Pressure [bar]	1	1	1	1	1
Feed flow [kg/h]	17 591	70 867.1	61 417.1	52.9	4 612.81
Fluid density [kg/m ³]	790	923	72	960	735
Residence time [h]	0.17	168	0.17	672	672
Disposition	Horizontal	Horizontal	Horizontal	Horizontal	Horizontal
Volume [m ³]	4.5	15 453	17.3	44.5	5 062
Length [m] (L)	2.8	43	4.4	6.1	30
Inner diameter [m] (D)	1.42	21.4	2.2	3.0	14.8
Outside diameter [m]	1.43	21.4	2.2	3.1	14.8
Thickness [mm]	5	5	5	5	5
Material	AISI 304	AISI 304	AISI 304	AISI 304	AISI 304
Sketch					

7.7. PUMPS

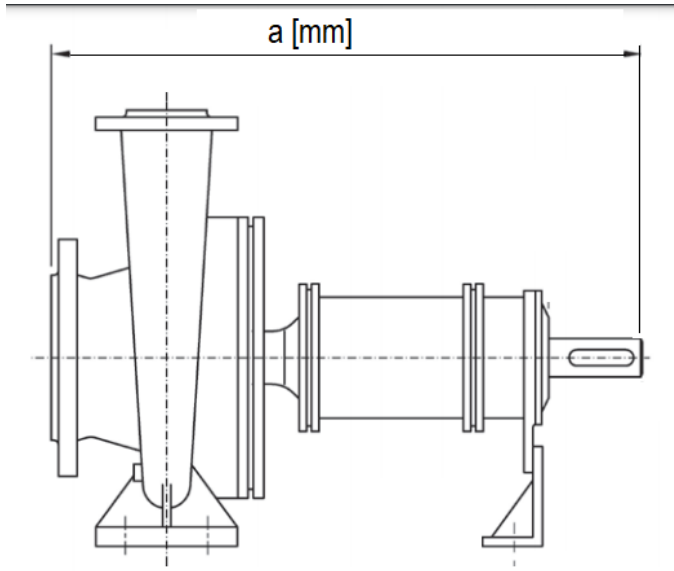
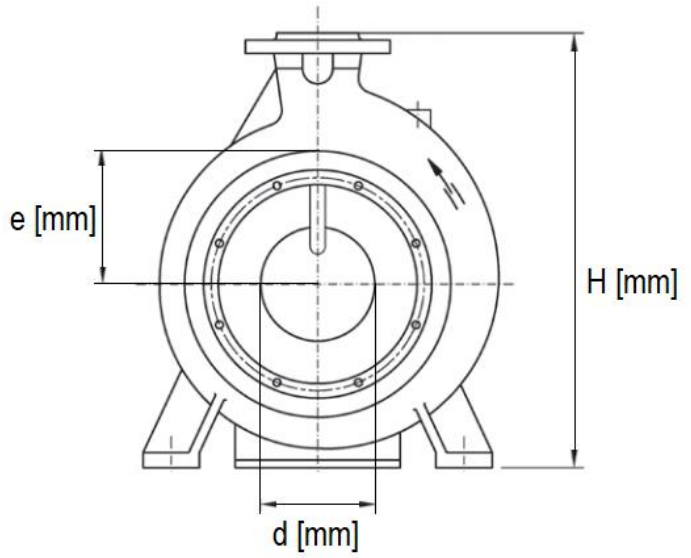
7 process pumps are designed, all of which are duplicated to guarantee the possible failure of one of them. For its design, it is first necessary to calculate the diameter of the pipes involved and their length. The procedure followed for the calculation of the pipes is defined in *Appendix VII*. In *Table 17* the most outstanding parameters of the pipes are tabulated, indicating according to the current to which they belong.

Table 17. Characteristic parameters of pipes

Stream [n°]	T [°C]	d [kg/m ³]	w [kg/h]	q [m ³ /h]	A _{MIN} [m ²]	NPS [INCH]	e [mm]	DN [mm]
3	20	1 089	93 200	85.6	0.024	8	8.18	200
4	20	1 089	93 200	85.6	0.024	8	8.18	200
7	32	1 082	82 000	75.8	0.021	8	8.18	200
10	32	1 082	83 804	77.4	0.022	8	8.18	200
14	32	996	1 926	1.9	0.001	2	3.91	60.3
15	32	996	1 926	1.9	0.001	2	3.91	60.3
20	0.1	1 009	76 197	75.5	0.021	8	8.18	200
21	0.04	1 009	76 197	75.5	0.021	8	8.18	200
31	45.8	790	17 581	22.2	0.006	4	6.02	114.3
32	45.8	790	17 581	22.2	0.006	4	6.02	114.3
33	45.8	790	12 478	15.8	0.004	3	5.49	88.9
34	45.8	790	5 103	6.5	0.002	2	3.91	60.3
44	44.4	722	61 417	85.0	0.024	8	8.18	200
45	44.4	722	61 417	85.0	0.024	8	8.18	200
46	44.4	722	32 171	44.5	0.012	5	6.55	141.3
47	44.4	722	29 246	40.5	0.011	5	6.55	141.3
49	44.4	722	29 193	40.5	0.011	5	6.55	141.3
50	44.4	722	29 193	40.5	0.011	5	6.55	141.3
55	77.6	735	4 613	6.3	0.002	2	3.91	60.3
58	77.6	735	4 613	6.3	0.002	2	3.91	60.3

Next, it moves on to the design of the pumps. Various parameters need to be calculated to be able to choose the ideal pump for the process from a catalog. In *Appendix VII* you will find the

Sketch



10. CONCLUSIONS

The plant is designed to obtain 4485 kg/h of bioethanol with a purity of 99.7% from sugar cane. For this, the three basic stages indicated in the literature are necessary, are discussed: food conditioning, fermentation, and ethanol purification.

The production process is not very profitable; therefore it is necessary to take into account many factors such as the variety of cane used, the location of the plant, the humidity, and the temperature of the environment.

A good variety of sugarcane to get the most out of the process is EC-05.

Building the same plant in Spain would be very complicated since the environmental conditions in Spain do not correspond to the optimal growth of sugar cane and manufacturing with an imported cane would be too expensive.

According to the biography, the optimal conditions to ferment sucrose are a pH of 4.5, a temperature of 32 °C, and a value between 6 to 10 °Bée.

The design of the plant gas considered a critical point, according to the bibliography, related to the concentration of ethanol: when the concentration of ethanol is greater than 10%, the *Saccharomyces Cerevisiae* becomes ineffective.

To separate CO₂ it is more profitable to use a flash separator than to directly use a distillation column and later use a partial condenser.

To obtain pure ethanol, it is necessary to use an extracting agent, MTBE in this case, since the ethanol-water mixture has an azeotrope at a concentration of 95.6% in ethanol.

11. RECOMMENDATIONS

For possible continuations of this work, it would be interesting to make a diagram of instrumentation and pipes, a lay-out and calculate the detailed cost of the plant.

Other options could be:

Make a comparison of the cost and the design of the equipment using different extraction agents.

Design a plant in which it takes advantage of the bagasse obtained in it to obtain more ethanol.

Compare the cost between fermentation and hydrolysis of sucrose using the same equipment or as two independent processes.

Search for other raw materials to achieve a profitable bioethanol production plant in Spain.

REFERENCES AND NOTES

- [1] *Etanol de caña de azúcar: el éxito de Brasil - América Latina y el Caribe*. América Latina y el Caribe. (2021). Retrieved 30 May 2021, from <https://www.scidev.net/america-latina/features/etanol-de-cao-de-azcar-el-xito-de-brasil/>.
- [2] Bioetanol: Proceso de fabricación y su importancia | Webscolar. Webscolar | Portal de recursos educativos, tareas, apuntes, monografías, ensayos. (2021). Retrieved 30 May 2021, from <https://www.webscolar.com/bioetanol-proceso-de-fabricacion-y-su-importancia>.
- [3] Sic.gov.co. (2021). Retrieved 30 May 2021, from https://www.sic.gov.co/sites/default/files/files/Propiedad%20Industrial/Boletines_Tecnologicos/BTBioetanol.pdf.
- [4] Repositorio.unican.es. (2021). Retrieved 30 May 2021, from <https://repositorio.unican.es/xmlui/bitstream/handle/10902/12178/RAF.pdf?sequence=1&isAllowed=y>.
- [5] *Azeótropo - Wikipedia, la enciclopedia libre*. Es.wikipedia.org. (2021). Retrieved 30 May 2021, from <https://es.wikipedia.org/wiki/Aze%C3%B3tropo#:~:text=Etanol%20y%20agua%20hierven%20a,hace%20a%2078.2%20%C2%B0C.&text=%E2%80%8B%20Se%20trata%20entonces%20de,d e%20la%20ley%20de%20Raoult>.
- [6] Atagua.org. (2021). Retrieved 30 May 2021, from https://www.atagua.org/presentaciones/XIVCongresoNacional2017/fabrica/composicion_quimica_dr_larrahondo.pdf.
- [7] Molienda de la Caña de Azúcar. Trapichsite.blogspot.com. (2021). Retrieved 30 May 2021, from <http://trapichsite.blogspot.com/2014/05/molienda-de-la-cana-de-azucar.html>.
- [8] (2021). Retrieved 30 May 2021, from <https://ecnautomation.com/recepcion-preparacion-y-molienda-de-la-cana-de-azucar/>.
- [9] Dspace.uce.edu.ec. (2021). Retrieved 30 May 2021, from <http://www.dspace.uce.edu.ec/bitstream/25000/2507/1/T-UCE-0017-68.pdf>.

- [10] mjr510, M. (2021). *DETERMINACIÓN ENZIMÁTICA DE SACAROSA - Monografias.com*. Monografias.com. Retrieved 30 May 2021, from <https://www.monografias.com/trabajos11/sara/sara.shtml>.
- [11] Bibing.us.es. (2021). Retrieved 30 May 2021, from <http://bibing.us.es/proyectos/abreproy/20046/fichero/Anexo%252FANEXO+4.pdf>.
- [12] Rinfi.fi.mdp.edu.ar. (2021). Retrieved 30 May 2021, from <http://rinfi.fi.mdp.edu.ar/xmlui/bitstream/handle/123456789/338/SMDiCarlo%2BFVPuyoi%2BRB%20VazquezWehrhahne-TFG-IQ-2019.pdf?sequence=1&isAllowed=y>.
- [13] Eprints.ucm.es. (2021). Retrieved 30 May 2021, from <https://eprints.ucm.es/id/eprint/2083/1/T18401.pdf>.
- [14] *El cultivo de la caña de azúcar*. Infoagro.com. (2021). Retrieved 30 May 2021, from <https://www.infoagro.com/herbaceos/industriales/canaazucar.htm#:~:text=Las%20zonas%20en%20Espa%C3%B1a%20de,plantaci%C3%B3n%20dura%20aproximadamente%205%20a%C3%B1os>.
- [15] d.o.o., Y. (2021). *Brasilía, Brasil - Información detallada del clima y previsión meteorológica mensual | Weather Atlas*. Weather Atlas. Retrieved 30 May 2021, from <https://www.weather-atlas.com/es/brasil/brasilia-clima#temperature>.
- [16] Servicios.laica.co.cr. (2021). Retrieved 30 May 2021, from <https://servicios.laica.co.cr/laica-cv-biblioteca/index.php/Library/download/fqyfCiuPLuLUIsKmjvrTokxyenLOJxc>.
- [17] *Alagoas - Wikipedia, la enciclopedia libre*. Es.wikipedia.org. (2021). Retrieved 30 May 2021, from <https://es.wikipedia.org/wiki/Alagoas>.
- [18] *Plantaciones más productivas. (2018), (Edición internacional)*. Retrieved 6 June 2021, from <https://revistapesquisa.fapesp.br/es/plantaciones-mas-productivas/>.
- [19] Cincae.org. (2021). Retrieved 30 May 2021, from <https://cincae.org/wp-content/uploads/2013/04/A%C3%B1o-15-1-y-2.pdf>.
- [20] Ullman's Encyclopedia of Industrial Chemistry, 7th edition. Volume 13, p. 364-365, "Ehanol".
- [21] Redalyc.org. (2021). Retrieved 30 May 2021, from <https://www.redalyc.org/pdf/1053/105312927004.pdf>.

- [22] Eprints.ucm.es. (2021). Retrieved 30 May 2021, from <https://eprints.ucm.es/id/eprint/2083/1/T18401.pdf>.
- [23] *Bomba centrífuga horizontal, Impulsor cerrado de proceso CPK-SY | Bombas centrífugas.Diseño-Fabricación-Customización.Emica Bombas* . Emicabombas.com. (2021). Retrieved 30 May 2021, from <https://www.emicabombas.com/es/productos/cpk-sy>.
- [24] Vladimir Castillo Uribe (2013) . Diseño y cálculo de un agitador de fluidos. Universidad del Bío-Bío, Chile,
- [25] Branan, C. (2005). Rules of thumb for chemical engineers. Gulf Professional Pub.
- [26] Apuntes de Transmisión de Calor. Dr. Ricard Torres i Castillo. (2021). Barcelona: Universitat de Barcelona
- [27] Ddd.uab.cat. (2021). Retrieved 30 May 2021, from https://ddd.uab.cat/pub/tfg/2017/183732/TFG_CHRORBEN_part11.pdf.
- [28] Apuntes de Circulacion de Fluidos. Joan Llorens Llacuna. (2021). Barcelona: Universitat de Barcelona
- [29] *Tabla schedule*. Es.slideshare.net. (2021). Retrieved 30 May 2021, from <https://es.slideshare.net/stopgabo/tabla-schedule>.
- [30] Lopei.files.wordpress.com. (2021). Retrieved 30 May 2021, from <https://lopei.files.wordpress.com/2010/06/practica-6.pdf>.
- [31] Ugr.es. (2021). Retrieved 30 May 2021, from <https://www.ugr.es/~aulavirtualpfciq/descargas/documentos/BOMBAS%20Y%20TUBERIAS.pdf>.
- [32] Industrialspec.com. (2021). Retrieved 5 June 2021, from <https://www.industrialspec.com/images/editor/chemical-compatibility-chart-from-ism.pdf>.

ACRONYMS

MTBE: Methyl tert-butyl ether

AISI: American Iron and Steel Institute

NPSH: Net Positive Suction Head

APPENDICES

APPENDIX I: PFD

#	1	2	3	4	5	6	7
Ethanol [kg/h]	0	0	0	0	0	0	0
Glucose [kg/h]	0	0	0	0	0	0	0
Saccharose [kg/h]	13 200	0	13 200	13 200	600	12 000	12 000
Water [kg/h]	77000	0	77 000	77 000	3 500	70 000	70 000
Fructose [kg/h]	0	0	0	0	0	0	0
Carbon dioxide	0	0	0	0	0	0	0
MTBE [kg/h]	0	0	0	0	0	0	0
Fiber	15 000	15 000	0	0	0	0	0
Impurities	3 000	0	3 000	30 00	3 000	0	0
Yeast	0	0	0	0	0	0	0
Total [kg/h]	108 200	15 000	93 200	93 200	7 100	82000	82 000
Pres [bar]	1	1	1	>1	1	1	<1
T [°C]	20	20	20	20	97	97	32

#	8	9	10	11	12	13	14
Ethanol [kg/h]	0	0	0	0	5756	0	0
Glucose [kg/h]	0	0	0	0	625	0	0
Saccharose [kg/h]	0	0	12 000	12 000	120	0	0
Water [kg/h]	17 767 080	17 767 080	70 000	70 000	69 375	0	0
Fructose [kg/h]	0	0	0	0	625	0	0
Carbon dioxide	0	0	0	0	5499	0	0
MTBE [kg/h]	0	0	0	0	0	0	0
Fiber	0	0	0	0	0	0	0
Impurities	0	0	0	0	0	0	0
Yeast	0	0	0	1804	1926	1926	1926
Total [kg/h]	17 767 080	17 767 080	82 000	83 804	83926	1926	1926
Pres [bar]	1	1	>1	>1	<1	<1	>1
T [°C]	10	15	32	32	32	32	32

#	15	16	17	18	19	20	21
Ethanol [kg/h]	0	0	5756	227	5528	5528	5528
Glucose [kg/h]	0	0	625	0	625	625	625
Saccharose [kg/h]	0	0	120	0	120	120	120
Water [kg/h]	0	0	69 375	301	69 073	69 073	69 073
Fructose [kg/h]	0	0	625	0	625	625	625
Carbon dioxide	0	0	5498	5274	225	225	225
MTBE [kg/h]	0	0	0	0	0	0	0
Fiber	0	0	0	0	0	0	0
Impurities	0	0	0	0	0	0	0
Yeast	122	1804	0	0	0	0	0
Total [kg/h]	122	1804	82 000	5803	76 197	76 197	76 197
Pres [bar]	>1	>1	<1	0	0	1	1
T [°C]	32	32	32	0	0	0	28

#	22	23	24	25	26	27	28
Ethanol [kg/h]	0	0	15 972	48	15 924	15 924	0
Glucose [kg/h]	0	0	0	0	0	0	0
Saccharose [kg/h]	0	0	0	0	0	0	0
Water [kg/h]	458 208	458 208	1490	3.7	1486	1486	461 361
Fructose [kg/h]	0	0	0	0	0	0	0
Carbon dioxide	0	0	346	175	170	170	0
MTBE [kg/h]	0	0	0	0	0	0	0
Fiber	0	0	0	0	0	0	0
Impurities	0	0	0	0	0	0	0
Yeast	0	0	0	0	0	0	0
Total [kg/h]	458 208	458 208	17 808	227	17 581	17 581	461 362
Pres [bar]	1	>1	1	1	1	1	1
T [°C]	140	130	46	46	46	46	1

#	29	30	31	32	33	34	35
Ethanol [kg/h]	0	15 924	15 924	11 302	4622	0	0
Glucose [kg/h]	0	0	0	0	0	785	160
Saccharose [kg/h]	0	0	0	0	0	151	31
Water [kg/h]	461 362	1486	1486	1055	431	86 572	17 651
Fructose [kg/h]	0	0	0	0	0	785	160
Carbon dioxide	0	170	170	121	49	0	0
MTBE [kg/h]	0	0	0	0	0	0	0
Fiber	0	0	0	0	0	0	0
Impurities	0	0	0	0	0	0	0
Yeast	0	0	0	0	0	0	0
Total [kg/h]	461 362	17 581	17 581	12 478	5103	88 294	18 002
Pres [bar]	<1	<1	>1	1	1	1	1
T [°C]	20.0	46	46	46	46	99	99

#	36	37	38	39	40	41	42
Ethanol [kg/h]	0	0	0	288	288	0	0
Glucose [kg/h]	625	0	0	0	0	0	0
Saccharose [kg/h]	120	0	0	0	0	0	0
Water [kg/h]	68 921	2 233 080	2 233 080	833	833	542 880	542 880
Fructose [kg/h]	625	0	0	0	0	0	0
Carbon dioxide	0	0	0	104	104	0	0
MTBE [kg/h]	0	0	0	60 192	60 192	0	0
Fiber	0	0	0	0	0	0	0
Impurities	0	0	0	0	0	0	0
Yeast	0	0	0	0	0	0	0
Total [kg/h]	70 292	2 233 080	2 233 080	61 417	61 417	542 880	542 880
Pres [bar]	1	3	<3	1	1	1	<1
T [°C]	98.8	140	130	44	44	10	20

#	43	44	45	46	47	48	49
Ethanol [kg/h]	288	288	151	137	0	137	137
Glucose [kg/h]	0	0	0	0	0	0	0
Saccharose [kg/h]	0	0	0	0	0	0	0
Water [kg/h]	833	833	436	397	49	347	347
Fructose [kg/h]	0	0	0	0	0	0	0
Carbon dioxide	104	104	54	49	0	49	49
MTBE [kg/h]	60 192	60 192	31 529	28 663	3	28 660	28 660
Fiber	0	0	0	0	0	0	0
Impurities	0	0	0	0	0	0	0
Yeast	0	0	0	0	0	0	0
Total [kg/h]	61 417	61 417	32 171	29 246	53	29 193	29 193
Pres [bar]	<1	>1	1	1	1	<1	>1
T [°C]	44	44	44	44	44	44	44

#	50	51	52	53	54	55	56	57
Ethanol [kg/h]	0	137	30 285	25 800	4485	0	0	4485
Glucose [kg/h]	0	0	0	0	0	0	0	0
Saccharose [kg/h]	0	0	0	0	0	0	0	0
Water [kg/h]	0	347	235	200	35	1 224 792	1 224 792	35
Fructose [kg/h]	0	0	0	0	0	0	0	0
Carbon dioxide	0	49	0	0	0	0	0	0
MTBE [kg/h]	96	28756	628	535	93	0	0	93
Fiber	0	0	0	0	0	0	0	0
Impurities	0	0	0	0	0	0	0	0
Yeast	0	0	0	0	0	0	0	0
Total [kg/h]	96	29 289	31 148	26 535	4613	1 224 792	1 224 792	4613
Pres [bar]	1	1	1	1	1	3	<3	1
T [°C]	55	44	78	78	78	140	130	78

APPENDIX II: FERMENTER DESIGN (R-211)

The first step is to choose the relationships between each dimension, the commonly used intervals between which the intermediate value has been chosen are indicated (*Table A1*) [24].

Table A1. List of dimensions [24]

Parameter Connexion	Connexion	Interval	Chosen value
Height of the liquid to the height of the reactor	H_L/H_T	0.7-0.8	0.75
Reactor height to tank diameter	H_T/D_T	1-2	1.5
Turbine diameter to tank diameter	D_a/D_t	0.3-0.5	0.4
Diameter of the baffles to the diameter of the tank	D_b/D_t	0.08-0.1	0.09
Turbine blade height to turbine diameter	W/D_a	0.2	0.2
Turbine blade width to turbine diameter	L/D_a	0.25	0.25
Distance from the aeration ring to the middle of the turbine	E/W	1	1
Distance between the turbine to the base of the reactor	C/D_t	0.333	0.333
Distance between the reactor wall and the baffle to the diameter of the reactor	f/D_t	0.02	0.02

Tank volume

The volume is calculated from the mass flow rate and the density of the fluid entering the fermenter. The values have been obtained from the simulation in *Aspen Plus V11*®.

$$V = \frac{m}{\rho} = \frac{82\,000 \frac{\text{kg}}{\text{h}}}{1\,0341.2 \frac{\text{kg}}{\text{m}^3}} = 79.3 \frac{\text{m}^3}{\text{h}}$$

Taking into account a residence time of 14 hours [20]:

$$V = 79.3 \frac{m^3}{h} \cdot 14 h = 1\,110.25 m^3$$

Applying a safety factor of 30% and knowing that it contains 2.2% yeast, the total volume is calculated [24]:

$$V = 1\,110.25 m^3 \cdot 1.322 = 1\,467.75 m^3$$

Height and diameter

The height and diameter are calculated applying the relationship indicated in the table and knowing that the shape of the reactor is conical [24]:

$$\frac{H}{D} = 1.5 \rightarrow H = 1.5 \cdot D$$

$$V = \frac{\pi}{4} \cdot D^2 \cdot H = 1.5 \cdot \frac{\pi}{4} \cdot D^3 = 1\,467.75 m^3$$

$$D = \sqrt[3]{\frac{4 \cdot 1\,338.2 m^3}{1.5 \cdot \pi}} = 10.76 m$$

$$H = 1.5 \cdot 10.76 = 16.14 m$$

Dome volume

It is calculated using the following equation and is replaced by the height of the dome (h) indicated in *Table 19* [24].

$$V_{dome} = \frac{\pi}{6} \cdot h \cdot (3 \cdot R^2 + h^2) = \frac{\pi}{6} \cdot h \cdot \left(3 \cdot \left(\frac{D}{2}\right)^2 + h^2 \right)$$

$$V_{dome} = \frac{\pi}{6} \cdot 0.120 \cdot 3 \left(\frac{10.76^2}{4} + 0.120^2 \right) = 5.45 m^3$$

Real Volume

$$V_{real} = V + V_{dome} = 1\,467.75 + 5.45 = 1\,473.2 m^3 \rightarrow 1\,500 m^3$$

Agitation

The 6 blades Rushton turbine has been chosen as it is typical for microbial reactors. In the reactors that use this turbine, a ratio between the diameter of the turbine and the diameter of the tank of 1/3 is used, therefore [24]:

$$\frac{D_a}{D} = 0.333 \rightarrow D_a = 0.333 \cdot 10.76 = 3.6 m$$

Knowing the diameter of the agitator, the height of the turbine blade (W) is calculated:

$$\frac{W}{D_a} = 0.2 \rightarrow W = 0.2 \cdot 3.6 = 0.72 m$$

And the width of the blade (L):

$$\frac{L}{D_a} = 0.25 \rightarrow L = 0.25 \cdot 3.6 = 0.9 \text{ m}$$

Also, the distance between the agitator and the base of the reactor (C) is calculated to optimize the process:

$$\frac{C}{D} = 0.333 \rightarrow C = 0.333 \cdot 10.76 = 3.6 \text{ m}$$

And the distance between the turbine and the oxygen supply ring (E):

$$\frac{E}{W} = 1 \rightarrow E = W = 0.72 \text{ m}$$

The useful height of the agitator (S) is given by the following formula:

$$S = \frac{2 \cdot D}{3} = \frac{2 \cdot 10.76}{3} = 7.2 \text{ m}$$

Baffles

To complete the agitation system, baffles will be added to break the circular movement generated by the agitator blades and thus generate greater turbulence and a better mixer.

Four baffles are placed 90° apart to facilitate agitation and facilitate cleaning of the system.

Motor

To improve agitation, a great turbulence is necessary. The turbulence is due to the currents being properly directed and can generate liquid velocity gradients. To carry it out, it is necessary to know the necessary power. To do this, it is first necessary to calculate the Reynolds number (Re) [24]:

$$Re = \frac{n \cdot D_a \cdot \rho}{\mu}$$

Being:

$$n: \text{agitator rotation speed} \rightarrow n = \frac{rpm}{60} = \frac{400}{60} = 6.67 \text{ rps}$$

D_a : turbine diameter

ρ : liquid density

μ : liquid viscosity

Substituting you get:

$$Re = \frac{6.67 \text{ rps} \cdot 3.5 \text{ m} \cdot 1034.1 \frac{\text{kg}}{\text{m}^3}}{0.000867 \text{ Pa}\cdot\text{s}} = 27\,844\,365$$

The result obtained shows that the regime is very turbulent. As the regime is turbulent and the reactor contains baffle plates, N_p is independent of the Reynolds number and the viscosity does not influence.

As a turbulent regime follows, the power number has a constant relationship through the following equation [24]:

$$N_{po} = \frac{P}{\rho \cdot n^3 \cdot D_a^5}$$

Being:

P: power required for agitation is defined by the following equation:

$$P = KT \cdot n^3 \cdot D_a^5 \cdot \rho$$

To find the value of KT is done following *Figure A1*.

Tipo de impulsor	KL	KT
Hélice paso cuadrado, tres palas	41,0	0,32
Hélice paso de 2, tres palas	43,5	1,00
Turbina, seis palas planas	71,0	6,30
Turbina, seis palas curvas	70,0	4,80
Turbina de ventilador, seis palas	70,0	1,65
Turbina dos palas planas	36,5	1,70
Turbina cerrada, seis palas curvas	97,2	1,08

Figure A1. KT value calculation according to type of impeller [24]

In this case, turbine, six flat blades, therefore, $KT = 6.30$.

$$P = 6.30 \cdot 6.67^3 \cdot 3.5^5 \cdot 1034.1 = 1\,015\,361\,778\,W = 1\,015\,362\,kW$$

Taking into account that the system will have three turbines but one of these will not be in contact with the fluid since its function will be to break the foam that appears, it will not need practically power. Therefore, the power used will be:

$$P_u = 2 \cdot 1\,015\,362 = 2\,030\,724\,kW$$

Taking into account an engine efficiency of 70%:

$$P_c = \frac{2\,030\,724}{0.7} = 2\,901\,034\,kW$$

Rounding up for possible problems and the presence of the third turbine, a power of 3 000 000 KW will be necessary.

APPENDIX III: FLASH DESIGN (S-311)

First, F_{LV} is calculated, which is the flow ratio from the densities and mass flows in the column. The simulation values are obtained in *Aspen Plus V11*® [25].

$$F_{LV} = \frac{L_{\text{másico}}}{V_{\text{másico}}} \cdot \sqrt{\frac{\rho_V}{\rho_L}} = \frac{76\,197.3 \text{ kg/h}}{5\,802.7 \text{ kg/h}} \cdot \sqrt{\frac{9.03 \cdot 10^{-5} \text{ g/cm}^3}{1.0091 \text{ g/cm}^3}} = 0.12$$

Next, K_{drum} is calculated, an empirical constant that depends on the flow rate and is necessary to calculate the allowed steam speed, that is, the maximum steam speed in the zone of maximum cross-sectional area [25].

$$K_{\text{drum}} = e^{[A+B \cdot \ln(F_{LV})+C \cdot \ln(F_{LV})^2+D \cdot \ln(F_{LV})^3+E \cdot \ln(F_{LV})^4]} = 2.0163 \frac{ft}{s} = 0.6146 \frac{m}{s}$$

Where A, B, C, D and E are empirical constants (Blackwell, 1984):

$$A = -1.877478097$$

$$B = -0.8145804597$$

$$C = -0.1870744085$$

$$D = -0.0145228667$$

$$E = -0.0010148518$$

The permitted steam velocity, U_P (m/s) is then calculated [25]:

$$U_P = K_{\text{drum}} \cdot \sqrt{\frac{\rho_L - \rho_V}{\rho_L}} = 0.12 \cdot \sqrt{\frac{1.0091 \frac{\text{g}}{\text{cm}^3} - 9.03 \cdot 10^{-5} \frac{\text{g}}{\text{cm}^3}}{1.0091 \frac{\text{g}}{\text{cm}^3}}} = 0.6145 \frac{\text{m}}{\text{s}}$$

And the passage area, A (m²) [25]:

$$A = \frac{V \cdot M_W}{U_P \cdot \rho_V} = \frac{141.5 \frac{\text{kmol}}{\text{h}} \cdot 19.96 \frac{\text{kg}}{\text{kmol}}}{3\,600 \frac{\text{s}}{\text{h}} \cdot 0.6145 \frac{\text{m}}{\text{s}} \cdot 0.009 \frac{\text{kg}}{\text{m}^3}} = 14.14 \text{ m}^2$$

Once the area has been calculated, the diameter, D (m) can be calculated according to the following equation:

$$D = \sqrt{\frac{4 \cdot A}{\pi}} = \sqrt{\frac{4 \cdot 14.14 \text{ m}^2}{\pi}} = 4.24 \text{ m}$$

And finally, the height, H (m):

$$\frac{H}{D} = 4 \rightarrow H = 4 \cdot D = 4 \cdot 4.24 \text{ m} = 16.97 \text{ m}$$

APPENDIX IV: EXCHANGERS DESIGN

I-114

The first step is to calculate is to define the fluid to be used to cool the fluid and in what temperature range the fluid is going to move. As you want to cool down from 97 °C to 32 °C, tap water is used which is heated from 10 °C to 20 °C. Water is chosen because it is the cheapest option, and it is situated at temperatures in which it is liquid.

Once this is defined, the flow of water required for cooling is calculated with the formula already indicated. The value of the heat exchanged is obtained from the simulation in *Aspen Plus V11*®.

$$w = \frac{5\,740 \text{ kW}}{4.18 \frac{\text{kJ}}{\text{kg}\cdot\text{K}}(20-10)} = 137.3 \frac{\text{kg}}{\text{s}}$$

The value obtained is necessary to be able to carry out the rigorous simulation and obtain all the design parameters of the equipment in Aspen together with the inlet temperature of both fluids. To carry out the simulation, it is necessary to define a third variable, in this case, the outlet temperature of the hot fluid.

With this defined, it is possible to obtain the simulation, but not the design of the equipment. To design the equipment, it is indicated what type of exchanger is, in this case, made of shell and tubes and which fluid goes through the shell and which through the tubes. In this case, it is chosen that the water (cold fluid) circulates through the tubes since this is the cleanest fluid, and thus cleaning will be facilitated. It is also defined B (cover and distributor in one piece) E (a casing passage) M (fixed tubular plate with type B distributor), B / M is chosen because very frequent

cleaning is not necessary inside the tubes. that water circulates, and it is the most economical and E why it is the most common. The number of Pitch chosen is the standard, the arrangement of the tubes chosen as well because it is the most common and the equipment material since this is the most compatible with all the fluids that circulate through the equipment [26].

Once the equipment has been designed, the final temperatures with which the required water flow has been calculated are not exact, this is due to pressure drops during the cooling process.

I-313

The first step is to calculate is to define the fluid to be used to heat the fluid and in what temperature range the fluid is going to move. As you want to heat from 0.36 °C to 28 °C, you use steam that cools from 140 °C to 130 °C.

Once this is defined, the flow of water required for cooling is calculated with the formula already indicated. The value of the heat exchanged is obtained from the simulation in *Aspen Plus V11*®.

$$w = \frac{2\,340\text{ kW}}{1.84 \frac{\text{kJ}}{\text{kg}\cdot\text{K}}(140-130)} = 127.2 \frac{\text{kg}}{\text{s}}$$

The value obtained is necessary to be able to carry out the rigorous simulation and obtain all the design parameters of the equipment in Aspen together with the inlet temperature of both fluids. To carry out the simulation, it is necessary to define a third variable, in this case, the cold fluid outlet temperature.

With this defined, it is possible to obtain the simulation, but not the design of the equipment. To design the equipment, it is indicated what type of exchanger is, in this case, made of shell and tubes and which fluid goes through the shell and which through the tubes. In this case, it is chosen that the water vapor (hot fluid) circulates through the tubes since this is the cleanest fluid and thus, cleaning will be facilitated. It is also defined B (cover and distributor in one piece) E (a casing passage) M (fixed tubular plate with type B distributor), B/M is chosen because very frequent cleaning is not necessary inside the tubes. that water circulates, and it is the most economical and E why it is the most common. The number of Pitch chosen is the standard, the arrangement of the tubes chosen as well because it is the most common and the equipment material since this is the most compatible with all the fluids that circulate through the equipment [26].

Once the equipment has been designed, the final temperatures with which the required water vapor flow rate has been calculated are not exact, this is due to pressure losses during the cooling process.

I-322

The first step is to calculate is to define the fluid to be used to cool the fluid and in what temperature range the fluid is going to move. As you want to cool down to go from vapor to liquid state, tap water is used that is heated from 10°C to 20°C. Water is chosen because it is the cheapest option, and it is situated at temperatures in which it is liquid.

Once this is defined, the flow of water required for cooling is calculated with the formula already indicated. The value of the heat exchanged is obtained from the simulation in Aspen Plus V11 ®.

$$w = \frac{5\,354\text{ kW}}{4.18 \frac{\text{kJ}}{\text{kg}\cdot\text{K}} (20-10)} = 128.1 \frac{\text{kg}}{\text{s}}$$

The value obtained is necessary to be able to carry out the rigorous simulation and obtain all the design parameters of the equipment in Aspen together with the inlet temperature of both fluids. To carry out the simulation, it is necessary to define a third variable, in this case, the fraction of steam at its outlet, since it is a partial condenser.

With this defined, it is possible to obtain the simulation, but not the design of the equipment. To design the equipment, it is indicated what type of exchanger is, in this case, made of shell and tubes and which fluid goes through the shell and which through the tubes. In this case, it is chosen that the water (cold fluid) circulates through the tubes since this is the cleanest fluid, and thus cleaning will be facilitated. It is also defined B (cover and distributor in one piece) E (a casing passage) M (fixed tubular plate with type B distributor), B / M is chosen because very frequent cleaning is not necessary inside the tubes. that water circulates, and it is the most economical and E why it is the most common. The number of Pitch chosen is the standard, the arrangement of the tubes chosen as well because it is the most common and the equipment material since this is the most compatible with all the fluids that circulate through the equipment [26].

Once the equipment has been designed, the final temperatures with which the required water flow has been calculated are not exact, this is due to pressure drops during the cooling process.

I-325

The first step is to calculate is to define the fluid to be used to heat the fluid and in what temperature range the fluid is going to move. As you want to heat the fluid to go from a liquid to a vapor, water vapor is used that cool from 140 °C to 130 °C.

Once this is defined, the flow of water required for cooling is calculated with the formula already indicated. The value of the heat exchanged is obtained from the simulation in *Aspen Plus V11*®.

$$w = \frac{11\,414\text{ kW}}{1.84 \frac{\text{kJ}}{\text{kg}\cdot\text{K}} (140-130)} = 620.3 \frac{\text{kg}}{\text{s}}$$

The value obtained is necessary to be able to carry out the rigorous simulation and obtain all the design parameters of the equipment in Aspen together with the inlet temperature of both fluids. To carry out the simulation, it is necessary to define a third variable, in this case, the heat exchanged by the equipment.

With this defined, it is possible to obtain the simulation, but not the design of the equipment. To design the equipment, it is indicated what type of exchanger is, in this case, made of shell and tubes and which fluid goes through the shell and which through the tubes. In this case, it is chosen that the water vapor (hot fluid) circulates through the tubes since this is the cleanest fluid and thus, cleaning will be facilitated. It is also defined B (cover and distributor in one piece) K (Kettle type vaporizer) U (U tubes), this type of design is chosen since it is the most common to vaporize the flow obtained per column foot in a column of distillation and the most economical. The number of Pitch chosen is the standard, the arrangement of the tubes chosen thus because it is the most common for the design of a Kettle type vaporizer and the equipment material since this is the most compatible with all the fluids that circulate through the team [26].

Once the equipment has been designed, the final temperatures with which the required water vapor flow rate has been calculated are not exact, this is due to pressure losses during the cooling process.

I-332

The first step is to calculate is to define the fluid to be used to cool the fluid and in what temperature range the fluid is going to move. As you want to cool down to go from vapor to liquid

state, tap water is used that is heated from 10°C to 20°C. Water is chosen because it is the cheapest option, and it is situated at temperatures in which it is liquid.

Once this is defined, the flow of water required for cooling is calculated with the formula already indicated. The value of the heat exchanged is obtained from the simulation in *Aspen Plus V11* ®.

$$w = \frac{6.305 \text{ kW}}{4.18 \frac{\text{kJ}}{\text{kg}\cdot\text{K}} (20-10)} = 150.8 \frac{\text{kg}}{\text{s}}$$

The value obtained is necessary to be able to carry out the rigorous simulation and obtain all the design parameters of the equipment in Aspen together with the inlet temperature of both fluids. To carry out the simulation, it is necessary to define a third variable, in this case, the fraction of steam at its outlet, since it is a partial condenser.

With this defined, it is possible to obtain the simulation, but not the design of the equipment. To design the equipment, it is indicated what type of exchanger is, in this case, made of shell and tubes and which fluid goes through the shell and which through the tubes. In this case, it is chosen that the water (cold fluid) circulates through the tubes since this is the cleanest fluid, and thus cleaning will be facilitated. It is also defined B (cover and distributor in one piece) E (a casing passage) M (fixed tubular plate with type B distributor), B / M is chosen because very frequent cleaning is not necessary inside the tubes. that water circulates, and it is the most economical and E why it is the most common. The number of Pitch chosen is the standard, the arrangement of the tubes chosen as well because it is the most common and the equipment material since this is the most compatible with all the fluids that circulate through the equipment [26].

Once the equipment has been designed, the final temperatures with which the required water flow has been calculated are not exact, this is due to pressure losses during the cooling process.

I-337

The first step is to calculate is to define the fluid to be used to heat the fluid and in what temperature range the fluid is going to move. As you want to heat the fluid to go from a liquid to a vapor, water vapor is used that cool from 140 °C to 130 °C.

Once this is defined, the flow of water required for cooling is calculated with the formula already indicated. The value of the heat exchanged is obtained from the simulation in *Aspen Plus V11* ®.

$$w = \frac{6\,260\text{ KW}}{1.84 \frac{\text{kJ}}{\text{kg}\cdot\text{K}} (140-130)} = 340.2 \frac{\text{kg}}{\text{s}}$$

The value obtained is necessary to be able to carry out the rigorous simulation and obtain all the design parameters of the equipment in *Aspen* together with the inlet temperature of both fluids. To carry out the simulation, it is necessary to define a third variable, in this case, the heat exchanged by the equipment.

With this defined, it is possible to obtain the simulation, but not the design of the equipment. To design the equipment, it is indicated what type of exchanger is, in this case, made of shell and tubes and which fluid goes through the shell and which through the tubes. In this case, it is chosen that the water vapor (hot fluid) circulates through the tubes since this is the cleanest fluid and thus, cleaning will be facilitated. It is also defined B (cover and distributor in one piece) K (Kettle type vaporizer) U (U tubes), this type of design is chosen since it is the most common to vaporize the flow obtained per column foot in a column of distillation and the most economical. The number of Pitch chosen is the standard, the arrangement of the tubes chosen thus because it is the most common for the design of a Kettle type vaporizer and the equipment material since this is the most compatible with all the fluids that circulate through the team ^[26].

Once the equipment has been designed, the final temperatures with which the required water vapor flow rate has been calculated are not exact, this is due to pressure losses during the cooling process.

APPENDIX V: DECANTER DESIGN (S-335)

The first parameter necessary to size the decanter is the time it takes for the mixture to separate properly. To do this, the following equation is followed [27]:

$$t = \frac{100 \cdot \mu}{\rho_A - \rho_B} = \frac{100 \cdot 0.2904 \text{ cP}}{960.0 \frac{\text{kg}}{\text{m}^3} - 721.6 \frac{\text{kg}}{\text{m}^3}} = 0.12 \text{ h} \rightarrow 7.2 \text{ min}$$

Being:

μ : Continuous phase viscosity (input)

ρ_A : heavy phase density

ρ_B : light phase density

Next, the volume necessary to carry out the separation is calculated from the volumetric flow at the inlet of the reactor.

$$V = 40.49 \frac{\text{m}^3}{\text{h}} \cdot 0.12 \text{ h} = 4.86 \text{ m}^3$$

Once the useful volume is obtained, 10% is added as a safety factor and an L/D = 5 ratio is used to calculate its dimensions, taking into account that the body is a cylinder with torispherical heads [27].

$$V = 1.1 \cdot 4.86 = 5.34 \text{ m}^3$$

$$V = \pi \cdot r^2 \cdot L = \frac{5}{8} \cdot \pi \cdot D^3 = 5.34 \rightarrow D = \sqrt[3]{\frac{8 \cdot 5.34}{5 \cdot \pi}} = 1.4 \text{ m} \rightarrow L = 5 \cdot 1.4 = 7 \text{ m}$$

To select the thickness, the API-650 standard is used and a value of 5 mm is selected and a diameter less than 15.2 m, it is obtained that the minimum thickness must be 4.76 mm. Taking into account that the material chosen is AISI-304.

APPENDIX VI: TANK DESIGN

T-323

First, the volume of product to be stored is calculated using the following equation:

Siendo:

$$V = \frac{m}{\rho} \cdot t \cdot F = \frac{17\,581 \frac{\text{kg}}{\text{h}}}{790.33 \frac{\text{kg}}{\text{m}^3}} \cdot 0.17 \text{ h} \cdot 1.2 = 4.54 \text{ m}^3$$

m: mass flow rate feeding the tank

ρ : fluid density

t: residence time

F: safety factor

A residence time of 10 minutes is considered because it is only a pass-through deposit and a safety factor of 1.2. Mass flow rate and density values are obtained from *Aspen Plus V11* ® simulation.

A 4: 1 ratio is used that relates the length of the tank to its radius. Taking into account that the shape is cylindrical, its length and radius can be calculated.

$$L = 4 \cdot r$$

$$V = \pi \cdot r^2 \cdot L = 4 \cdot \pi \cdot r^3 = 4.54 \text{ m}^3 \rightarrow r = \sqrt[3]{\frac{4.54}{4 \cdot \pi}} = 0.71 \text{ m}$$

$$L = 4 \cdot r = 0.71 \text{ m} \cdot 4 = 2.84 \text{ m}$$

To select the thickness, the API-650 standard is used and a value of 5 mm is selected since, for tanks stored at atmospheric pressure, at a maximum temperature of 93.3 °C and a diameter less than 15.2 m, it is obtained that the minimum thickness must be 4.76 mm. Taking into account that the material chosen is AISI-304.

T-326

To calculate the volume, a residence time of 1 week and a safety factor of 1.2 are considered. Mass flow rate and density values are obtained from *Aspen Plus V11*® simulation. For the calculation of the dimensions, the same relationships are used as for the T-323.

$$V = \frac{m}{\rho} \cdot t \cdot F = \frac{70\,867.1 \frac{\text{kg}}{\text{h}}}{923.32 \frac{\text{kg}}{\text{m}^3}} \cdot 168 \text{ h} \cdot 1.2 = 15\,453.3 \text{ m}^3$$

$$r = \sqrt[3]{\frac{15\,453.3}{4 \cdot \pi}} = 10.7 \text{ m} \rightarrow L = 4 \cdot 10.7 \rightarrow 42.9 \text{ m}$$

To select the thickness, the API-650 standard is used and a value of 5 mm is selected since, for tanks stored at atmospheric pressure and a diameter less than 15.2 m, the minimum thickness must be 4.76 mm. Taking into account that the material chosen is AISI-304.

T-333

To calculate the volume, a residence time of 10 minutes is considered because it is only a pass-through deposit and a safety factor of 1.2. Mass flow rate and density values are obtained from *Aspen Plus V11*® simulation. For the calculation of the dimensions, the same relationships are used as for the T-323.

$$V = \frac{m}{\rho} \cdot t \cdot F = \frac{61\,417.3 \frac{\text{kg}}{\text{h}}}{722.24 \frac{\text{kg}}{\text{m}^3}} \cdot 0.17 \text{ h} \cdot 1.2 = 17.3 \text{ m}^3$$

$$r = \sqrt[3]{\frac{17.3}{4 \cdot \pi}} = 1.1 \text{ m} \rightarrow L = 4 \cdot 1.1 \rightarrow 4.4 \text{ m}$$

To select the thickness, the API-650 standard is used and a value of 5 mm is selected since, for tanks stored at atmospheric pressure, at a maximum temperature of 93.3 °C and a diameter less than 15.2 m, it is obtained that the minimum thickness must be 4.76 mm. Taking into account that the material chosen is AISI-304.

T-336

To calculate the volume, a residence time of 1 month (28 days) and a safety factor of 1.2 are considered. Mass flow rate and density values are obtained from *Aspen Plus V11*® simulation. For the calculation of the dimensions, the same relationships are used as for the T-323.

$$V = \frac{m}{\rho} \cdot t \cdot F = \frac{52.94 \frac{kg}{h}}{960 \frac{kg}{m^3}} \cdot 672 h \cdot 1.2 = 44.5 m^3$$

$$r = \sqrt[3]{\frac{44.5}{4 \cdot \pi}} = 1.52 m \rightarrow L = 4 \cdot 1.52 \rightarrow 6.1 m$$

To select the thickness, the API-650 standard is used and a value of 5 mm is selected since, for tanks stored at atmospheric pressure, at a maximum temperature of 93.3 °C and a diameter less than 15.2 m, it is obtained that the minimum thickness must be 4.76 mm. Taking into account that the material chosen is AISI-304.

T-339

To calculate the volume, a residence time of 1 month (28 days) and a safety factor of 1.2 are considered. Mass flow rate and density values are obtained from *Aspen Plus V11* ® simulation. For the calculation of the dimensions, the same relationships are used as for the T-323.

$$V = \frac{m}{\rho} \cdot t \cdot F = \frac{4612.81 \frac{kg}{h}}{734.9 \frac{kg}{m^3}} \cdot 672 h \cdot 1.2 = 5\,061.6 m^3$$

$$r = \sqrt[3]{\frac{5\,061.6}{4 \cdot \pi}} = 7.4 m \rightarrow L = 4 \cdot 7.4 \rightarrow 30 m$$

To select the thickness, the API-650 standard is used and a value of 5 mm is selected since, for tanks stored at atmospheric pressure, at a maximum temperature of 93.3 °C and a diameter less than 15.2 m, it is obtained that the minimum thickness must be 4.76 mm. Taking into account that the material chosen is AISI-304.

APPENDIX VII: PIPE AND PUMP DESIGN

PIPELINES

First, the volumetric flow rate is calculated according to the following equation:

$$q \left[\frac{m^3}{h} \right] = \frac{w}{\rho}$$

Being:

w: mass flow [kg/h]

ρ : density [kg/m³]

Next, the minimum area is calculated. For this, it is necessary to know the state of the fluid, in all cases it is liquid, and that for liquids the target speed is 3 600 m/h [28]. With this, the minimum area is obtained according to the following equation:

$$A_{min} [m^2] = \frac{q}{v}$$

Taking into account that a pipe has a circular shape, the minimum diameter is obtained:

$$A = \pi \cdot r^2 \rightarrow d_{min} = \sqrt{\frac{4 \cdot A}{\pi}}$$

Once the minimum diameter has been obtained, the diameter of the pipe is approximated to establish a standard value, which is always higher than the minimum calculated. With the NPS in inches, the value of the thickness and the nominal diameter is obtained following the bibliography [29].

Pumps

Primeramente, se calcula la velocidad del fluido según la siguiente ecuación:

$$v \left[\frac{m}{s} \right] = \frac{4 \cdot q}{3\,600 \cdot \pi \cdot d^2}$$

Being:

q: Volumetric flow rate [m³/h]

d: nominal diameter [m]

Next, the Reynolds number is calculated:

$$Re = \frac{d \cdot v \cdot \rho}{\mu}$$

Being:

d: nominal diameter [m]

v: velocity [m/s]

ρ : density [kg/m³]

μ : viscosity [Pa·s]

Values not previously calculated are obtained from *Aspen Plus V11*® simulation.

Calculate the coefficient of friction, f. This parameter depends on the type of flow and in all cases, as the Reynolds number is higher than 4,000, it is calculated by following the following equation, which comes from the Moody diagram ^[30].

$$f = 0.0055 \left[1 + \left[20\,000 \cdot \frac{e}{d} + \frac{10^6}{Re} \right]^{1/3} \right]$$

Being:

e: thickness [m]

d: nominal diameter [m]

Next, the pressure drop is calculated ^[31]:

$$H[m] = \left(\frac{4 \cdot f \cdot L}{d} \right) \cdot \frac{v^2}{2 \cdot g}$$

Being:

f: coefficient of friction

L: equivalent length [m]

d: nominal diameter [m]

v: velocity [m/s]

The equivalent length is not only the length of the pipe but also includes the pressure drop that occurs through an elbow or when passing through a valve. Following the bibliography, the equivalent length is calculated taking into account that each pump contains a valve at the inlet, and at the outlet, that the equipment at the inlet contains another valve and most of them also at the outlet. All the valves used are globe type.

Next, the suction pressure (P_A) in the inlet pipes to the pump is calculated following the following equation ^[31]:

$$P_A = P_1 + (h_r - Z_1) \cdot (\rho \cdot g)$$

Being:

P_1 : pressure at the beginning of the pipe [Pa]

Z_1 : initial height [m]

h_r : friction loss, calculated using Darcy's equation $\rightarrow h_r = f \cdot \frac{L}{D} \cdot \frac{v^2}{2 \cdot g}$

And for the second section of the pipe, the impulse pressure (P_B) ^[31]:

$$P_B = P_2 + (h_r + Z_1) \cdot (\rho \cdot g)$$

Being:

P_2 : desired pressure at the end of the pipe [Pa]

Z_2 : final height [m]

h_r : friction loss

To calculate the manometric height, it is done using the following equation ^[31]:

$$\Delta h = \frac{P_B - P_A}{\rho \cdot g} + h_r + h_a$$

Being:

h_a : friction losses in the different accessories found in the pipe

It is calculated using the following expression:

$$h_a = \sum K \cdot \frac{v^2}{2 \cdot g}$$

Being:

v : fluid velocity [m/s]

K : coefficient of friction of accessories, being 0.4 for 90 ° elbows and 10 for globe valves

Finally, the $NPSH_{available}$ is calculated using the following equation:

$$NPSH_{dis} = \frac{P_1 - P_v}{\rho \cdot g} + Z_1 - h_r - h_a$$

Being:

P_1 : pressure at the beginning of the pipe

P_v : Vapor pressure is calculated by averaging the vapor pressure of each compound involved in the composition of the fluid by its vapor pressure at the temperature at which it circulates.

h_f : friction losses

h_a : los from accessories

Once all the parameters have been obtained, the pump is chosen from the catalog. For this, the manometric head and the volumetric flow are necessary. Once located in the graph, the pump to which it corresponds is chosen and the dimensions indicated by the manufacturer are obtained.

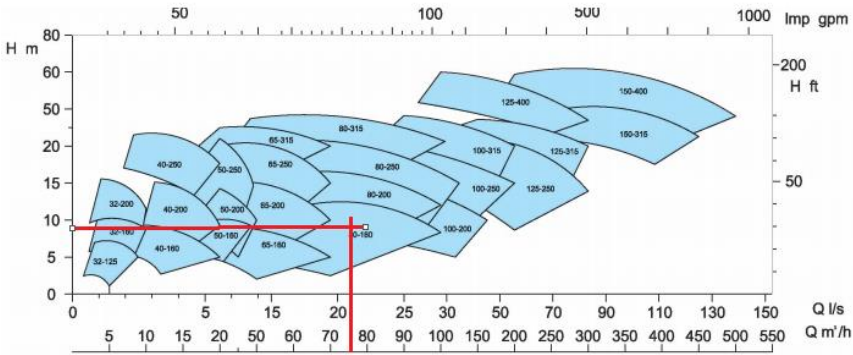


Figure A2. Pump selection B-112-a/b [23]

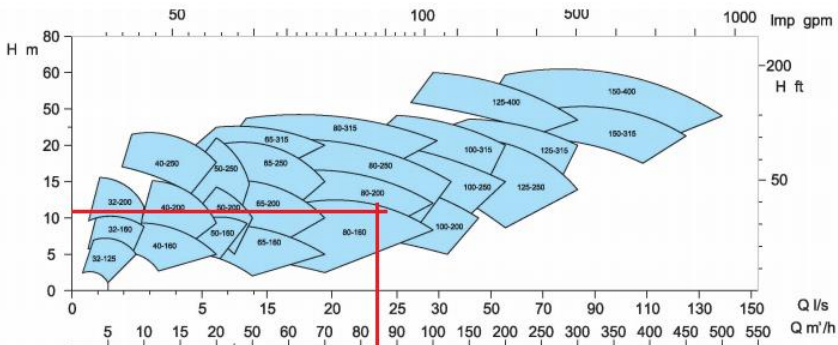


Figure A3. Pump selection B-115-a/b [23]

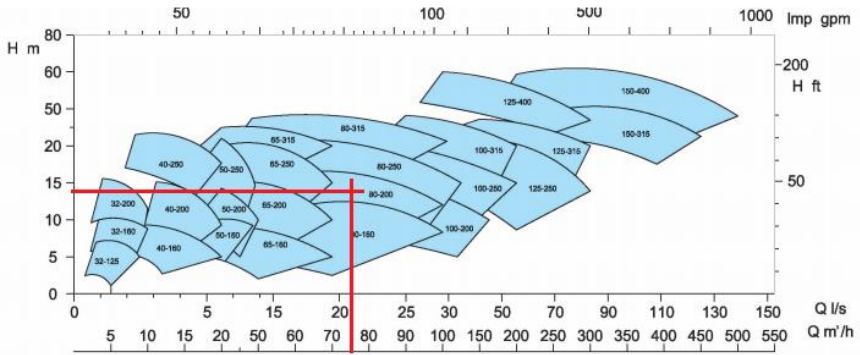


Figure A4. Pump selection B-312-a/b [23]

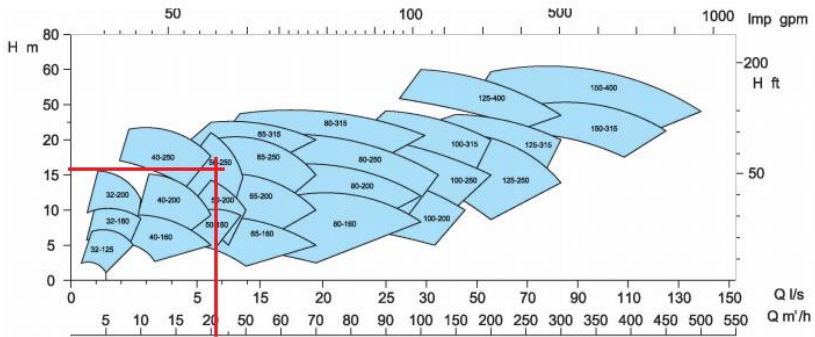


Figure A5. Pump selection B-324-a/b [23]

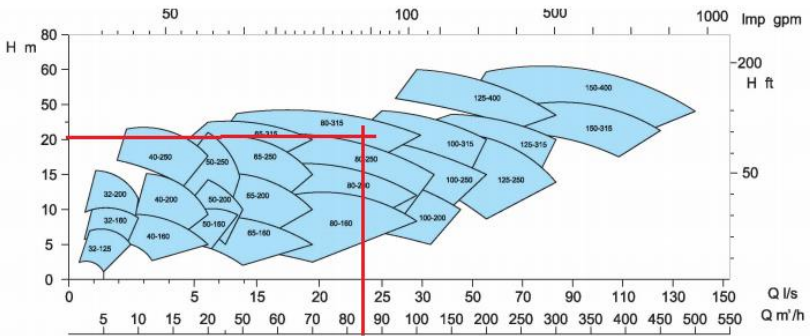


Figure A6. Pump selection B-334-a/b [23]

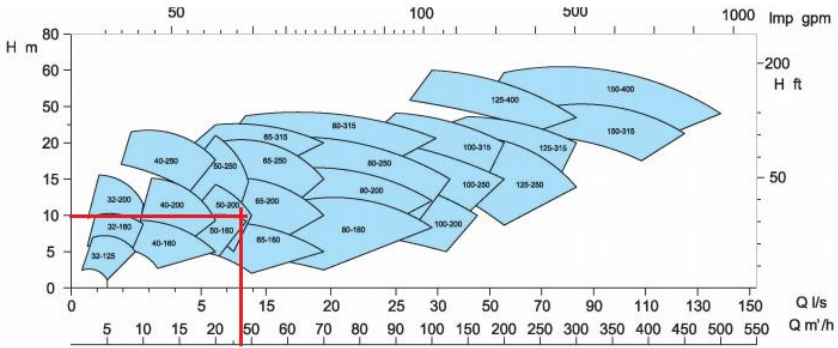


Figure A7. Pump selection B-337-a/b [23]

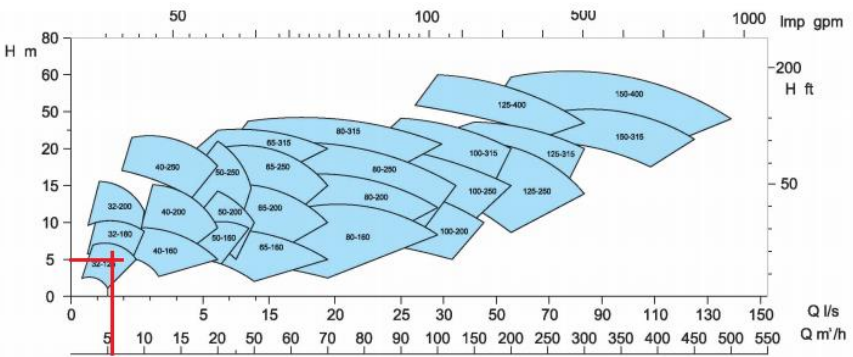


Figure A8. Pump selection B-339-a/b [23]

The dimensions of each pump are calculated according to Figure 16 and Figure 17.

Bridas Bomba / Pump flanges / Brides pompe DIN 2533 PN-16										
DN	25	32	40	50	65	80	100	125	150	200
Df	115	140	150	165	185	200	220	250	285	340
Kf	85	100	110	125	145	160	180	210	240	295
gf	68	78	88	102	122	138	158	188	212	268
Zf	4	4	4	4	4	8	8	8	8	12
lf	14	18	18	18	18	18	18	18	23	23

Figure A9. Pump dimensions 1 [23]

Tamaño / Size Taille	Medidas de bomba / Pump dimensions Mesures de pompe						Medidas de pata / Foot dimensions / Mesures de pied											Extremo del eje / Shaft end / Extrémité de l'arbre					
	DN1	DN2	a	f	h ₁	h ₂	b	m ₁	m ₂	m ₃	n ₁	n ₂	d ₁	s ₁	s ₂	w	i	c	x	d _{ax}	l	t	u
32-125	50	32	80	360	112	140	50	100	70	45	190	140	14	8	12	260	23	100	100	22	50	26,9	8
32-160	50	32	80	360	132	160	50	100	70	45	240	190	14	8	14	260	23	100	100	22	50	26,9	8
32-200	50	32	80	360	160	180	50	100	70	47	240	190	14	8	14	260	23	100	100	22	50	26,9	8
40-160	65	40	80	360	132	160	50	100	70	45	240	190	14	8	14	260	23	100	100	22	50	26,9	8
40-200	65	40	100	360	160	180	50	100	70	47	265	212	14	8	14	260	23	100	100	22	50	26,9	8
40-250	65	40	100	360	180	225	65	125	95	47	320	250	14	8	16	260	23	100	100	22	50	26,9	8
40-315	65	40	125	470	200	250	65	125	95	47	345	280	14	8	18	370	23	130	100	32	80	35,3	10
50-160	80	50	100	360	160	180	50	100	70	45	265	212	14	8	14	260	23	100	100	22	50	26,9	8
50-200	80	50	100	360	160	200	50	100	70	45	265	212	14	8	14	260	23	100	100	22	50	26,9	8
50-250	80	50	125	360	180	225	65	125	95	47	320	250	14	8	14	260	23	100	100	22	50	26,9	8
65-160	100	65	100	360	160	200	65	125	95	45	280	212	14	8	15	260	23	100	100	22	50	26,9	8
65-200	100	65	100	360	180	225	65	125	95	47	320	250	14	8	16	260	23	100	100	22	50	26,9	8
65-250	100	65	125	470	200	250	80	160	120	47	360	280	18	8	18	340	23	130	140	32	80	35,3	10
65-315	100	65	125	470	225	280	80	160	120	47	400	315	18	8	18	340	23	130	140	32	80	35,3	10
80-160	125	80	125	360	180	225	65	125	95	47	320	250	14	8	15	260	23	100	140	22	50	26,9	8
80-200	125	80	125	470	180	250	65	125	95	47	345	280	14	8	16	340	23	130	140	32	80	35,3	10
80-250	125	80	125	470	225	280	80	160	120	47	400	315	18	8	18	340	23	130	140	32	80	35,3	10
80-315	125	80	125	470	250	315	80	160	120	52	400	315	18	12	18	340	26	130	140	32	80	35,3	10
100-200	125	100	125	470	200	280	80	160	120	47	360	280	18	8	16	340	23	130	140	32	80	35,3	10
100-250	125	100	140	470	225	280	80	160	120	47	400	315	18	8	18	340	23	130	140	32	80	35,3	10
100-315	125	100	140	470	350	315	80	160	120	52	400	315	18	12	18	340	26	130	140	32	110	35,3	10
125-250	150	125	140	470	250	355	80	160	120	52	400	315	18	12	18	340	26	130	140	32	80	35,3	10
125-315	150	125	140	530	280	355	100	200	150	52	500	400	23	12	20	370	26	160	140	42	110	45,1	12
125-400	150	125	140	530	315	400	100	200	150	52	500	400	23	12	20	370	26	160	140	42	110	45,1	12
150-315	200	150	160	530	315	400	100	200	150	52	550	450	23	12	22	370	26	160	140	42	110	45,1	12
150-400	200	150	160	530	315	450	100	200	150	52	550	450	23	12	22	370	26	160	140	42	110	45,1	12

Figure A10. Pump dimensions 2 [23]

And the desired parameters are obtained according to Figure A11. Only the most prominent parameters are found in the specification sheet, but all the measurements indicated in the figure are obtained.

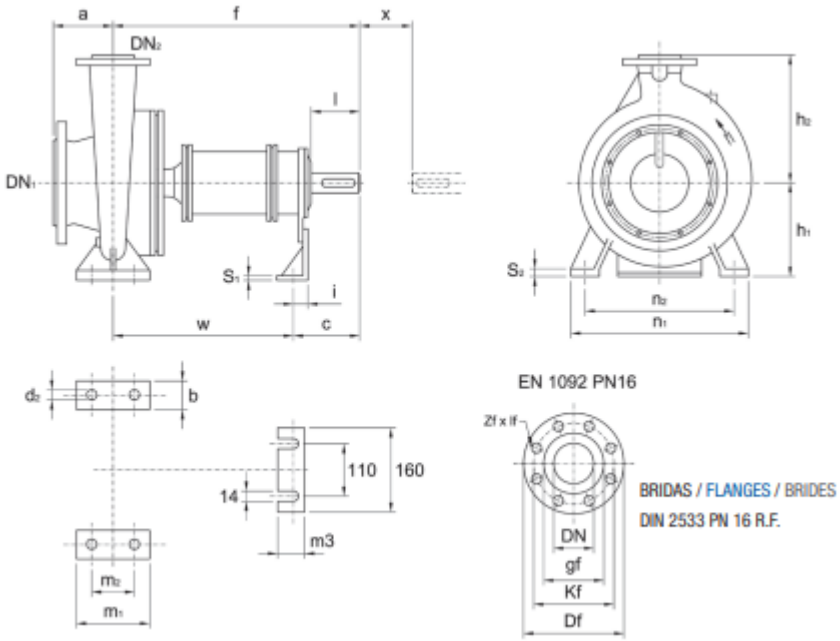


Figure A11. Pump diagram to obtain dimensions [23]

APPENDIX VIII. MATERIAL SELECTION

To avoid problems of corrosion or other properties due to the chosen material, it is chosen taking into account the compatibility of each compound involved in the process. AISI 304 is chosen for all equipment since it is more compatible with all compounds as can be seen in the *Figure A12* [32].

	304 Stainless Steel	316 Stainless Steel	ABS Plastic	Acetal, POM	Acrylic (PMMA)	Aluminum	Brass	Bronze	Buna N (Nitrile)	Cast Iron	Copper	CPVC	EPDM
Alcohols: Ethyl	A	A	B	A	C	B	A	A	C	B	A	B	A
Glucose	A	A	B	A	A	A	A	N/A	A	A	A	A	A
Water, Distilled	A	A	B	B	A	A	A	A	A	D	B	A	A
Butyl Ether	B	A	N/A	D	D	A	N/A	N/A	B	N/A	N/A	D	D
Carbon Dioxide, wet	A	A	B	A	A	A	A	A	A	D	A	A	B

Figure A12. Material compatibility