UNIVERSIDADE DE SANTIAGO DE COMPOSTELA

ESCOLA TÉCNICA SUPERIOR DE ENXEÑARÍA

Grado en Ingeniería Química

FINAL DEGREE PROJECT

PRODUCTION FACILITY OF POLILACTIC ACID FROM LACTIC ACID

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Year 2018/2019

GENERAL INDEX

DOCUMENT I

Descriptive Report

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1. Objective

This document focuses on a facility design for the production of polylactic acid (PLA). The main product, PLA, which is a biopolymer, is obtained from 80% purity lactic acid with a polymerization reaction. This facility can operate continuously during 330 days per year and have a fixed production capacity of 50000 tons/year.

Among the goals, another is: to obtain by Sofía Estévez Rivadulla the degree in Chemical Engineering given by the "Universidade de Santiago de Compostela".

2. Introduction

2.1 Background

The worldwide plastics manufacturing has been estimated in 335 million tons in 2016 from which 60 million were produced in Europe. The plastics production has been, since the early nature of its productive activities in 1950, 8.3 billion tons.

Spain is the fourth country in the European Union demanding plastics. The 50% of this plastics are finally disposed in landfills which must increase their capacity in order to accommodate the plastic wastes. In this context and with the intention of reducing wastes, the biopolymers were developed. The poly (lactic acid) is one of the best known and produced biodegradable polyesters due to its physical properties and cost which are optimal for several applications. [1]

The present project proposes an introduction to this biopolymer production. The interaction between relatively new concepts and with social and industrial awareness are shown: technological progress, security and environmental protection.

The poly (lactic acid) is produced from lactic acid, which was isolated in 1780 and introduced in the market in 1881. It was used only for medical application until 1997 when the Cargill Dow LLC Company pushed the market for the development of patents allowing the production of low cost PLA in volume production. So today, the PLA has multiple applications, some of which are intended to the textile field, the agricultural field, the biomedicine and the packaging.

2.2 Justification for the project/scope

The project scope will depend on its maturity level, which is linked to the information provided. Therefore, this final grade report must be seen as a document of basic engineering. All information required in order to achieve the project´s objectives is included in this section.

- Analysis of the viability of the project considering: legislation framework, market and economic aspects, reaction pathway possibilities and technical feasibility.
- Description of the facilities location, the facilities itself, the process, the equipment and the environment of the site (with an environmental impact assessment).
- Heat and Material Balances.
- Instrumentation/control system.
- Equipment design.

  - Security in the facilities, safety data sheets of the substances and Safety and Health Studies.
  - Discipline drawings: Process Flow Diagram (PFD), Piping & Instrumentation Diagram (P&ID), Site location plan, Location map, Implementation plan, and Equipment design plan.
  - General and specific solicitation documents for construction works.
  - General budget.

3. Standards, legislation and design codes

This project´s section introduces the main applicable laws, standards and design codes. The regulations are classified according to the following mayor topics: construction, environment, and industrial hygiene and security.

3.1 Normative framework

3.1.1 Technical norms and procedure instruction for building works

- Technical Building Code (Royal Decree 314/2006).

3.1.2 Electricity regulations

- Low Voltage Electrotechnical regulation and Complementary Technical Instructions (CTI) 01 to 51.

3.1.3 Safety and Health standards

- Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission

Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC.

- Regulation (EU) 2016/425 of the European Parliament and of the Council of 9 March 2016 on personal protective equipment and repealing Council Directive 89/686/EEC.
- Regulation for Annoying, Unhealthy, Harmful and Dangerous Activities (RAMINP).
- Basic Study of Hygiene and Security in on Construction Works (EBS).

3.2 Legislative framework

3.2.1 General legislation

- Law 21/1992 of 12 July, industry.
- Royal Decree 2060/2008 of 12 December which approves the regulation of pressure equipment and its Complementary Technical Instructions.
- Royal Legislative Decree 2/2015 of 23 October 2015 approving the consolidated text of the Workers' Statute Act.

3.2.2 Legislation related to building construction

3.2.2.1 General building construction legislation

- Law 38/1999 of 5 November 1999 on the Organization of building construction.
- Law 5/2015 of 25 July by the Valencia Regional Government regarding Land Use, Urban Planning and Landscaping of the Valencia Community.
- Royal Decree 256/2016 of 10 June, along with the Instruction on Structural Cement (RC-16).
- Royal Decree 314/2006 of 17 March approving the Technical Building Code.
- Royal Decree 1247 / 2008 of 18 July which approves the statement of structural concrete (Ehe-08).

3.2.2.2 Electric legislation

- Royal Decree 842/2002 of 2 August approving the Low Voltage Electrotechnical Regulations.

3.2.3 Legislation related to industrial health and hygiene

3.2.3.1 Legislation to prevention and control of risks at work

- Directive (EU) 2017/2102 of the European Parliament and of the Council of 15 November 2017 amending Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment.
- Law 31/1995 of 8 November on the Prevention of Occupational Risks.
- Law 54/2003 of 12 December on the reform of the regulatory framework for the Prevention of Occupational Risks.
- Royal Decree 39/1997 of 17 January approving the Regulations on prevention services.
- Royal Decree 780/1998 of 30 April amending Royal Decree 39/1997, of 17 January, approving the regulation of prevention services.
- Royal Decree 604/2006 of 19 May amending Royal Decree 39/1997, of 17 January, approving the Prevention Services Regulations.
- Royal Decree 598/2015 of 3 July amending Royal Decree 39/1997, of 17 January, approving the Regulations on prevention services.
- Royal Decree 899/2015 of 9 October amending Royal Decree 39/1997, of 17 January, approving the Prevention Services Regulations.
- Royal Decree 1196/2003 of 19 September by adopting the basic guideline for civil protection and planning to control the risk of major accidents involving dangerous substances.
- Royal Decree 656/2017 of 23 June approving the Regulations for the Storage of Chemical Products and their Complementary Technical Instructions MIE APQ 0 to 10.
- Royal Decree 833/1998 of 20 July approving the Regulation for the implementation of Law 20/1986, Basic on Toxic and Hazardous Waste.
- Royal Decree 840/2015 of 21 September approving measures to control the risks inherent in serious accidents involving dangerous substances.
- Royal Decree 2267/2004 of 3 December approving the Regulation on fire safety in industrial establishments.

3.2.3.2 Health and safety legislations

- Council Directive 89/654/EEC of 30 November 1989 concerning the minimum safety and health requirements for the workplace (first individual directive within the meaning of Article 16 (1) of Directive 89/391/EEC)
- Council Directive 89/656/EEC of 30 November 1989 on the minimum health and safety requirements for the use by workers of personal protective equipment at the workplace (third individual directive within the meaning of Article 16 (1) of Directive 89/391/EEC).
- Council Directive 92/58/EEC of 24 June 1992 on the minimum requirements for the provision of safety and/or health signs at work (ninth individual Directive within the meaning of Article 16 (1) of Directive 89/391/EEC).
- Royal Decree 286/2006 of March 10 on the Protection of the Health and Safety of workers from the risks related to exposure to noise.
- Royal Decree 330/2009 of 13 March amending Royal Decree 1311/2005, of 4 November, on the protection of the health and safety of workers against risks arising or that may arise from exposure to mechanical vibrations.
- Royal Decree 337/2010 of 19 March amending Royal Decree 39/1997, of 17 January, approving the Prevention Services Regulations.
- Royal Decree 1109/2007, of 24 August, implementing Law 32/2006 of 18 October regulating subcontracting in the construction sector.
- Royal Decree 374/2001 of 6 April 2001 on the protection of the health and safety of workers from the risks related to chemical agents at work.
- Royal Decree 485/1997 of 14 April on minimum requirements for safety and health signs at work.
- Royal Decree 486/1997 of 14 April 1997 laying down minimum safety and health requirements in the workplace.
- Royal Decree 487/1997 of 14 April 1997 on minimum safety and health requirements relating to the manual handling of loads involving risks, in particular dorsolumbar, for workers.
- Royal Decree 488/1997 of 14 April 1997 on minimum safety and health requirements relating to working with equipment including display screens.
- Royal Decree 1627/1997 of 24 October establishing the minimum safety and health requirements for construction sites.
- Royal Decree 614/2001 of 8 June on minimum provisions for the protection of the health and safety of workers against electrical risk.

- Royal Decree 773/1997 of 30 May 1997 on minimum safety and health requirements for the use by workers of personal protective equipment.
- Royal Decree 1215/1997 of 18 July 1997 laying down the minimum safety and health requirements for the use of work equipment by workers.
- Royal Decree 1311/2005 of 4 November on the protection of the health and safety of workers against the risks derived or that may derive from exposure to mechanical vibrations.
- Royal Decree 1627/1997 of 24 October establishing the minimum safety and health requirements for construction sites.
- Royal Decree 1072/2015 of 27 November amending Royal Decree 2200/1995, of 28 December, approving the Infrastructure Regulations for Quality and Industrial Safety.
- Royal Decree 1407/1992 of 20 November 1992 regulating the conditions for the marketing and free movement within the Community of personal protective equipment.
- Royal Decree 1879/1996 of 2 August on the composition of the National Commission on Safety and Health at work.
- Royal Decree 2200/1995 of 28 December approving the Infrastructure Regulations for Quality and Industrial Safety.
- Royal Decree 513/2017 of 22 May approving the Regulation on Fire Protection Installations.
- Royal Decree 577/1982 of 17 March 1982 regulating the structure and powers of the National Institute for Safety and Hygiene at Work.
- Royal Decree 485/1997 of 14 April on minimum provisions on safety and health signs at work.

3.2.3.3 Hygiene legislations

- Royal Decree 665/1997 of 12 May 1997 on the protection of workers against risks related to exposure to carcinogens at work.
- Royal Decree 374/2001 of 6 April 2001 on the protection of the health and safety of workers against risks related to chemical agents at work.

3.2.4 Legislation related to the environment

3.2.4.1 Legislation related to environmental footprint

- Directive 2010/75/EU of the European Parliament and of the Council of 24 November 2010 on industrial emissions (integrated pollution prevention and control).
- Directive 2011/92/EU of the European Parliament and of the Council of 13 December 2011 on the assessment of the effects of certain public and private projects on the environment.
- Directive 2014/52/EU of the European Parliament and of the Council of 16 April 2014 amending Directive 2011/92/EU on the assessment of the effects of certain public and private projects on the environment.
- Law 26/2007 of 23 October amending Environmental Liability.
- Law 11/2014, of 3 July, amending Law 26/2007, of 23 October, amending Environmental Liability.
- Law 6/2014 of 25 July on prevention and environmental quality control activities in the Valencia Community.
- Law 21/2013 of 9 December, environmental assessment.
- Royal Decree 508/2007 of 20 April 2007 which regulates the supply of information about emissions of the EPRTR Regulation and the environmental authorizations included.
- Royal Decree 773/2017 of 28 July amending various royal decrees on industrial products and emissions.
- Royal Decree 815/2013 of 18 October approving the Regulation on industrial emissions and the development of Law 16/2002 of 1 July on integrated pollution prevention and control.
- Royal Legislative Decree 1/2016 of 16 December approving the consolidated of the integrated pollution prevention and control Law.
- Environmental Assessment Act 21/2013 of 9 December 2013.

3.2.4.2 Legislation related to atmospheric emissions

- Directive 2008/50/EC of the European Parliament and of the Council of 21 May 2008 on ambient air quality and cleaner air for Europe.
- Law 22/1983 of 21 November 1983 on the protection of the atmospheric environment.
- Law 34/2007 of 15 November on air quality and protection of the atmosphere.

- Law 9/2018 of 5 December amending Law 21/2013 of 9 December on environmental assessment, Law 21/2015 of 20 July amending Law 43/2003 of 21 November on forestry and Law 1/2005 of 9 March regulating the greenhouse gas emission allowance trading scheme.
- Royal Decree 39/2017 of 27 January amending Royal Decree 102/2011 of 28 January on improving air quality.
- Royal Decree 102/2011 of 28 January on the improvement of air quality.
- Royal Decree 678/2014 of 1 August amending Royal Decree 102/2011 of 28 January on the improvement of air quality.
- Royal Decree 547/1979 of 20 February amending Annex IV of Decree 833/1975 of 6 February developing the Law on the Protection of the Atmospheric Environment.
- Decree 833/1975 of 4 February, elaborated upon by Law 38/1972 of 22 December on the protection of the atmospheric environment.

3.2.4.3 Legislation related to waters and wastewaters

- Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy.
- Royal Decree 1290/2012, of 7 September, amending the Regulation of the Public Hydraulic Domain, approved by Royal Decree 849/1986, of 11 April, and Royal Decree 509/1996, of 15 March, implementing Royal Decree-Law 11/1995, of 28 December, establishing the rules applicable to the treatment of urban waste water.
- Royal Legislative Decree 1/2001 of 20 July approving the consolidated text of the Water Law.
- Royal Decree-Law 11/1995 of 28 December establishing the rules applicable to the treatment of urban waste water.
- Royal Decree-Law 4/2007 of 13 April amending the revised text of the Water Law, approved by Royal Legislative Decree 1/2001, of 20 July.
- Decision No 2455/2001/EC of the European Parliament and of the Council of 20 November 2001 establishing the list of priority substances in the field of water policy and amending Directive 2000/60/EC (Text with EEA relevance).

3.2.4.4 Legislation related to waste disposal and soils

- Directive 2008/98/EC of the European Parliament and of the Council of 19 November 2008 on waste and repealing certain Directives.
- Law 5/2013 of June 11th, amending Law 16/2002 of July 1st, on integrated pollution prevention and control and Law 22/2011 of July 28th, on waste and contaminated soils.
- Royal Decree 105/2008 of 1 February which regulates the production and management of construction and demolition waste.
- Order MAM/304/2002 of 8 February publishing waste recovery and disposal operations and the European waste list.

3.2.4.5 Legislation related to noise pollution

- Directive 2000/14/EC of the European Parliament and of the Council of 8 May 2000 on the approximation of the laws of the Member States relating to the noise emission in the environment by equipment for use outdoors.
- Directive 2002/49/EC of the European Parliament and of the Council of 25 June 2002 relating to the assessment and management of environmental noise.
- Law 37/2003 of 17 November on Noise.
- Law 7/2002 of 3December of the Generalitat Valenciana of protection against noise pollution.
- Royal Decree 212/2002 of 22 February regulating noise emissions in the environment due to certain machines for outdoor use.
- Royal Decree 1513/2005 of 16 December implementing Law 37/2003 of 17 November, on Noise, in relation to the evaluation and management of environmental noise.
- Decree 104/2006 of 14 July of the Consell of noise pollution planning and management.
- Decree 266/2004 of 3 December of the Consell of the Generalitat establishing preventive and corrective standards for noise pollution in activities, facilities, buildings, works and services.

3.3 Design codes

- A.S.M.E (American Society of Mechanical Engineers)
- T.E.M.A (American Tubular Exchanger Manufacturers Association)

- U.N.E (“Una Norma Española”)
- D.I.N (“Deutsches Institut für Normung”)
- A.P.I (American Petroleum Institute)
- BS (British Standards)

4. Market research

4.1 Scope of the study

In this market study a preliminary analysis is provided to point out some common characteristics. The product manufactured in the facility design for this project is to be placed in this market.

The bioplastics market is introduced and referred to during this study to enhance the importance of PLA, its production capacity and price through several years, its market evolution and projections. Furthermore, trade between different continents, within the European Union and national trade characteristics shall be explained. Lastly, some key factors that influence the poly (lactic acid) market and the main competitors are included.

In addition, a similar analysis is also made of the raw material, lactic acid. From this last analysis the PLA production and demand may be deduced.

4.2 Poly (lactic acid) market definition

The global poly (lactic acid) market is currently growing. This increase is a reflection of the biodegradable plastics demand rise, increasing urbanization, awareness of sea plastic pollution, and an increase demand in sectors related to the automobile or packaging industries. Besides, the electric and electronic industry will increase the biopolymer use in coming years.

Apart from the previously explained, an appropriate favorable context that stimulates the growth and development of the bioplastics market is shown: increasing environmental concern related to the plastics landfill disposal, new government regulations facilitating the market growth and prevention of oil consumption needed for other more required purposes. But even so, this growth is tempered by the bioplastics price, especially poly (lactic acid) (PLA from now on), which are higher than the conventional plastics of petrochemical base. In 2017, the 38.7% of the plastics were already biodegradable and the remaining 61.3% were bio-based or non-biodegradable. In figure 1 are shown some plastics, including biodegradable and non-biodegradable plastics, and their relative significance according to the total global production capacity.

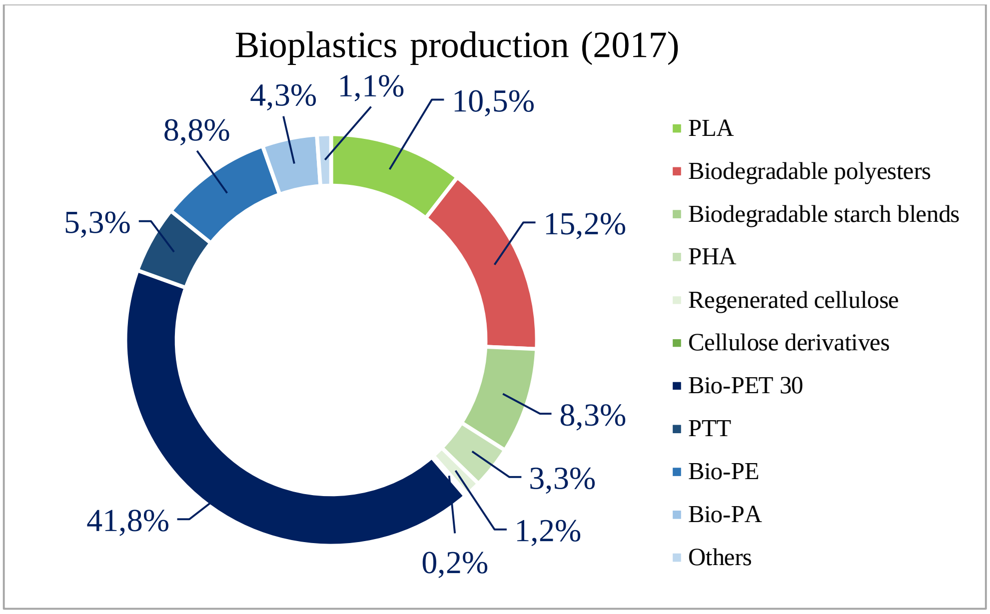


Figure 1. Significant bioplastics production in 2017. [2]

Figure 1 shows that PLA, the project product, represents around the 10.2% of the bioplastics total production, thus being the biodegradable plastic putting the highest pressure on the market.

The global poly (lactic acid) market is divided into five well-known regions: Asia, Europe, South America, North America, Africa and Oceania. In this sense, the market study to be considered in the following sections take the previously mentioned regions as basis. [3]

4.3 Poly (lactic acid) production and consumption

The poly (lactic acid) production capacity, in the context of the bioplastics trade, is continuously growing. In 2014 the bioplastics production capacity was of around 1.7 million metric tons. In 2017, this value was approximately 2.3 million metric tons and is expected to rise to 4.3 million in 2022. From this total value of production capacity, in 2017, a 10.5% of the production was for PLA (such as figure 1 illustrates).

The market was also valued in dollars. In 2017, the bioplastic market was valued at around US$ 6.05 billion and, being more specific, the PLA market was valued at US$ 698.27 million. [4]

Another important issue to be taken into account is the PLA consumption/demand. United States consumed about half of the total PLA in 2014. It is therefore, the largest consumer of this substance. In 2017, United States consumed 74,319 metric tons of PLA. Europe is the second largest market when considering the consumption level. This is because in Europe there is a favorable legal framework and awareness about environmental protection among consumers.

4.4 Raw materials and products prices

4.4.1 Lactic acid prices

The lactic acid prices fluctuate constantly and depend on the market behavior, although they also depend on the lactic acid purity. There is lactic acid with food quality having purities of 50% and 88% and with technological quality having weight compositions of 88%. The food quality lactic acid has range prices between 1.40 US$/kg and 1.90$US/kg which corresponds to a 50% and an 88% fraction weight. The lactic acid of technological quality has prices around 1.60 US$/kg. [5]

4.4.2 Poly (lactic acid) prices

Figure 2 shows lactic acid prices from january to october in 2017. According to what is shown in the figure, the lactic acid price remains practically stable over the year and the prices change in a range from 1,910 US$/ton to 5,950 US$/ton depending on the market region. The asiatic region shows the highest PLA market prices, whereas in North America the prices are lower.

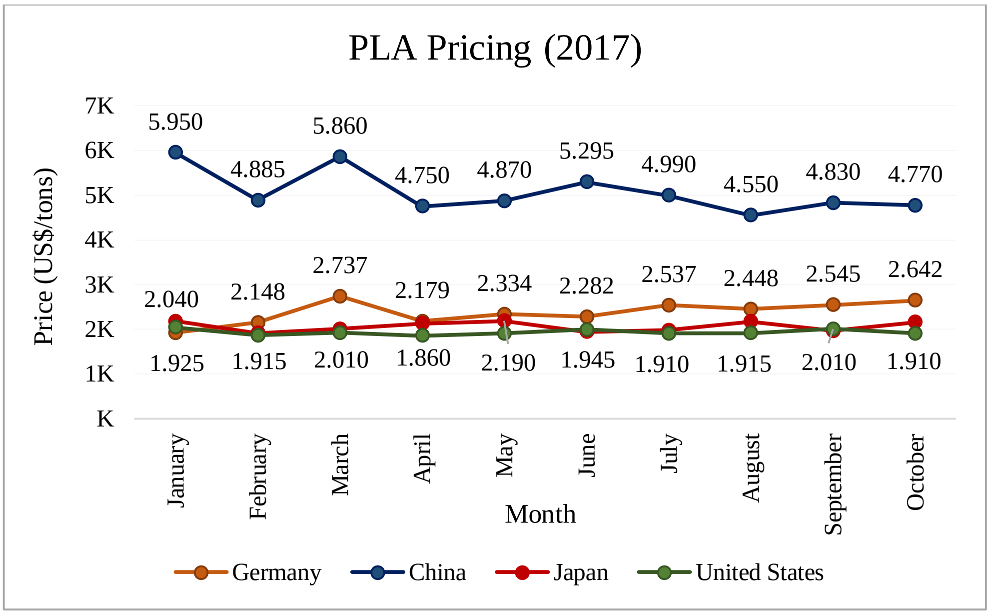


Figure 2. Poly (lactic acid) prices in 2017. [6]

4.5 Medium to long- term trend

The long-term PLA market is growing fast. However, this growth is being tempered by land constraints for the raw material production, lactic acid. The global lactic acid market was valued in US$ 1.83 billion in 2015 and is expected to rise up to US$ 6.25 billion by 2022 with an annual growth of 19.1% from 2015 to 2022. This market growth will be affected by lactic acid applications in plastics production, among other things. [7]

The medium to long-term PLA market trend is influenced by the biopolymer global market. By the end of 2025 the market might reach a value of US$ 7.77 billion with an annual growth of 14.0% since 2017 to 2025. [8]

With regard to the PLA production capacities, figure 1 and 3 can be compared. It is expected that PLA market rises and its production capacity becomes 18.7% from the total production capacity anticipated, with regard to the 10.5% already shown for 2017.

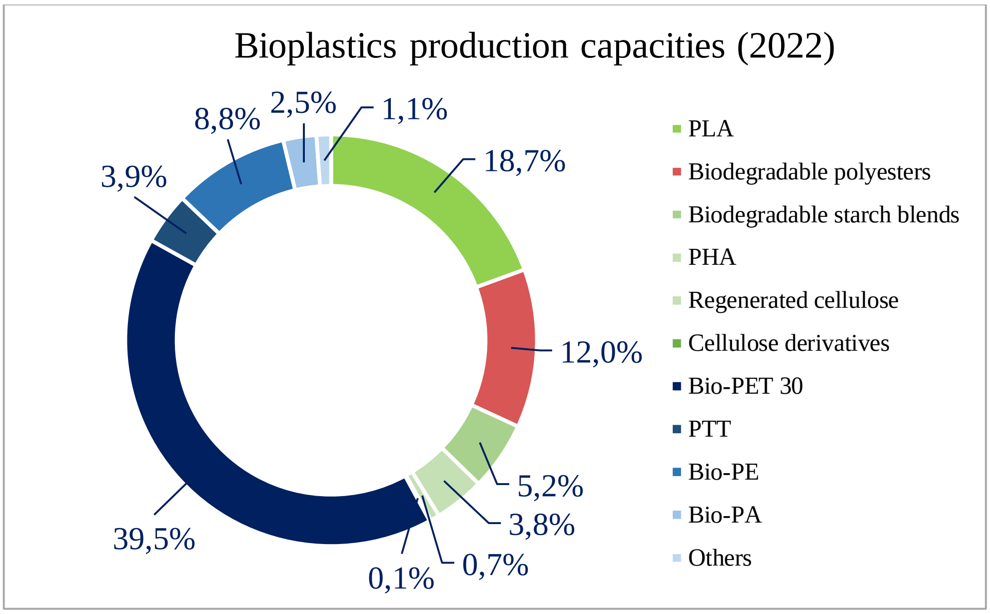


Figure 3. Some bioplastics production capacities significance in 2022. [2]

It is within this context in where the medium long-term PLA market growth can be explained. According to this, in 2023, the global PLA market will be valued in US$ 2,091.29 million with an annual growth of 20.06% since 2017 to 2023.

4.6 Factors involve in the market evolution

The global PLA market evolution depends on these aspects:

- **Restrictions:** PLA high price, if compared with other non-biodegradable plastics.
- **Key drivers:** New government policies which are favorable to PLA market increase, new environmentally-friendly regulations for waste management, increase concern about human health, increasing of the packaging industry applications and new investigations in order to discover new bio-based plastics.
- **Opportunities in the market:** In relationship with groundbreaking applications and with the high growth of the PLA global market in the Asiatic countries.
- **Challenges in the market:** Difficulties for the segregation and processing bioplastic when seeking for a circular economy, fluctuations in the raw material prices, applications and limitations when using the biopolymer and limitations in some regulations.
- **Some key developments:** The industry sector related to the polymer production is changing constantly. New applications, patents, agreement between undertakings and policies are making the market evolve. According to this, some developments which have influence in the market evolution can be named. In January 2018, Bengdu-based BBCA Group enter into agreement with Glactic Company on a project for the production of 100,000 metric tons of PLA. In June 2017, NatuWorks sign a contract for the D-lactic acid production with the Plaxica´s Optipure chemical technology. [9]

4.7 Trade flows

4.7.1 Lactic acid (raw material)

4.7.1.1 Exportations

Europe is the largest lactic acid exporter region in the world. In 2017, lactic acid has been exported for a total value of US$ 333 million and according to the information shown graphically in figure 4, Europe has dominated the exportations since 2005, although already had the control of the lactic acid world market since a few years before 2005.

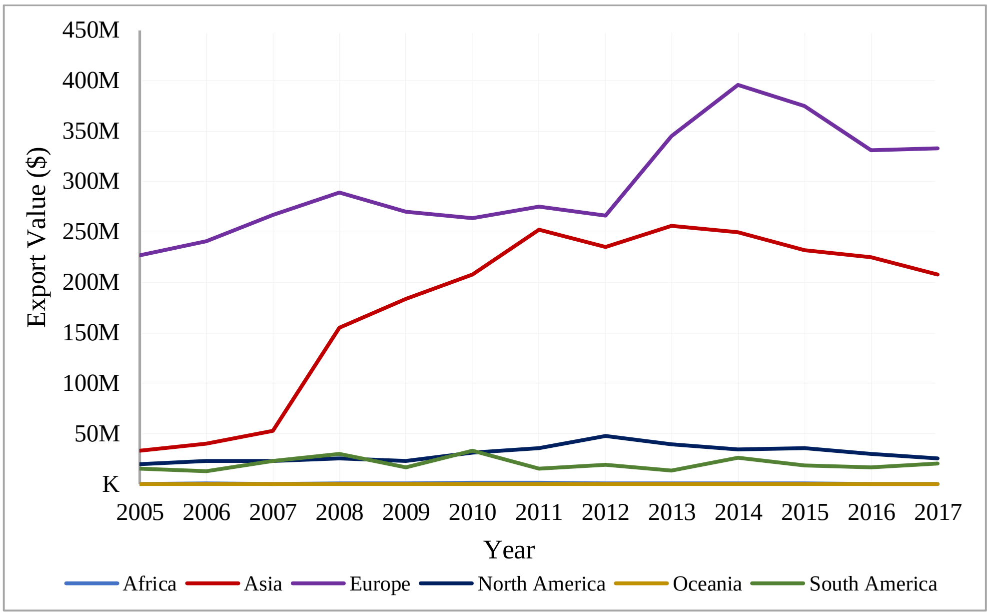


Figure 4. Lactic acid export trends around the world. [3]

The exportations value has risen in Europe since 2005. There has been a market increase of US$ 106 million since 2005 to 2017, although since 2014 (year at which the greatest lactic acid exportation value has been reached) the exportations have been suffering a reduction in value.

Asia is the second largest lactic acid exporter region. Since 2007, the Asian market has suffered a boost, which leads to a rise of the exportation values in US$ 175 million. This increase happening between 2005 and 2017 is higher that the increase experienced by Europe. In 2017, the lactic acid exportation values became US$ 208 million for this region.

Africa, America and Oceania have exported lactic acid in 2017 for a total value of US$ 491,000, 46 million and 361,000 and the exportations trend has not undergone enormous changes since 2005.

In Africa, South Africa and Kenya highlight as some of the largest exporter countries. In Asia can be outlined Thailand and China, in North America are United States and Mexico, in South America are Brazil and Argentina, in Oceania are New Zealand and Australia and in Europe are Netherlands and Spain.

In Europe, the total value of the lactic acid exportations is around US$ 133 million for Netherlands and is US$ 66.9 million for Spain. There are other large lactic acid exporters in Europe like Belgium, Luxembourg, Germany and France. In figure 5 are shown the exportation value trend for all the previously named countries since 2005. In the figure can be seen an increase of the exportations until 2014, year at which the total exportation value started its reduction.

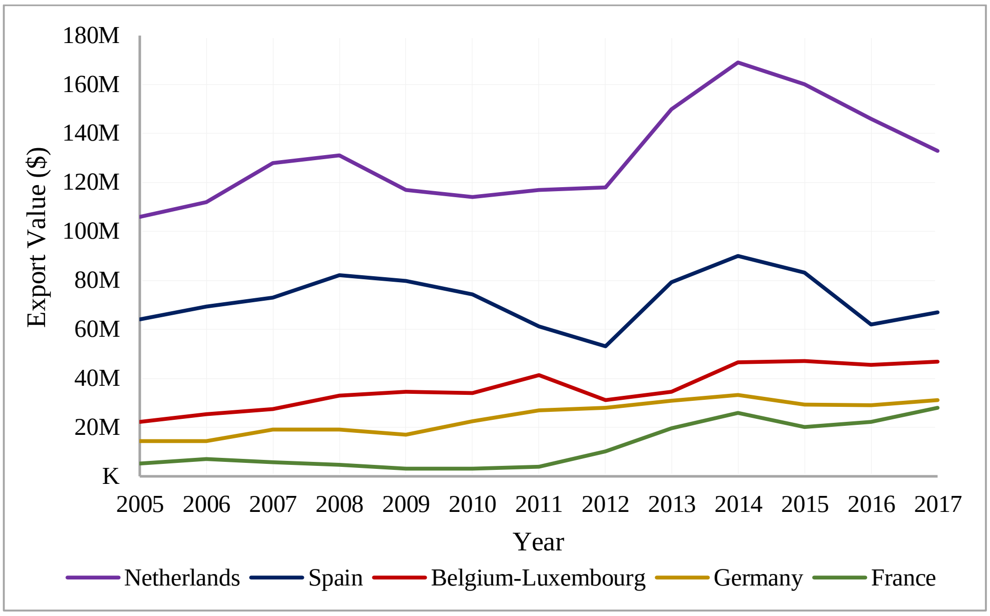


Figure 5. Lactic acid export trends for the main European export countries. [3]

In figure 6 is shown the fraction of lactic acid exported by the main European export countries. Netherlands export the 40% of the total lactic acid exportations made in Europe and Spain exports a 20%. It is therefore that in this figure are indicated some illustrative percentages and their relationship with total value of the exportations made, in dollars.

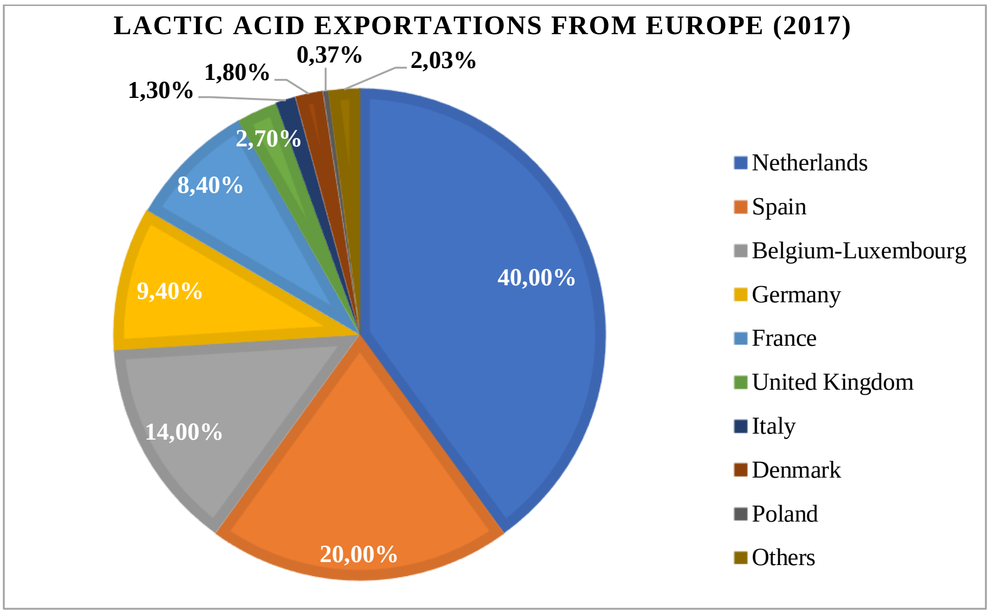


Figure 6. Lactic acid exportations in Europe, 2017. [3]

As previously explained, Spain exported lactic acid to a total of US$ 66.9 million. The 55% were exportations made to other European countries. America received the 25.1% of the lactic acid, Asia, the 15% and Africa, the remaining 4.8%. Some of the countries to which Spain export the greatest part of the lactic acid are: Italy, Netherlands, United States, México and France. The figure 7 shows some of the lactic acid exporter countries.

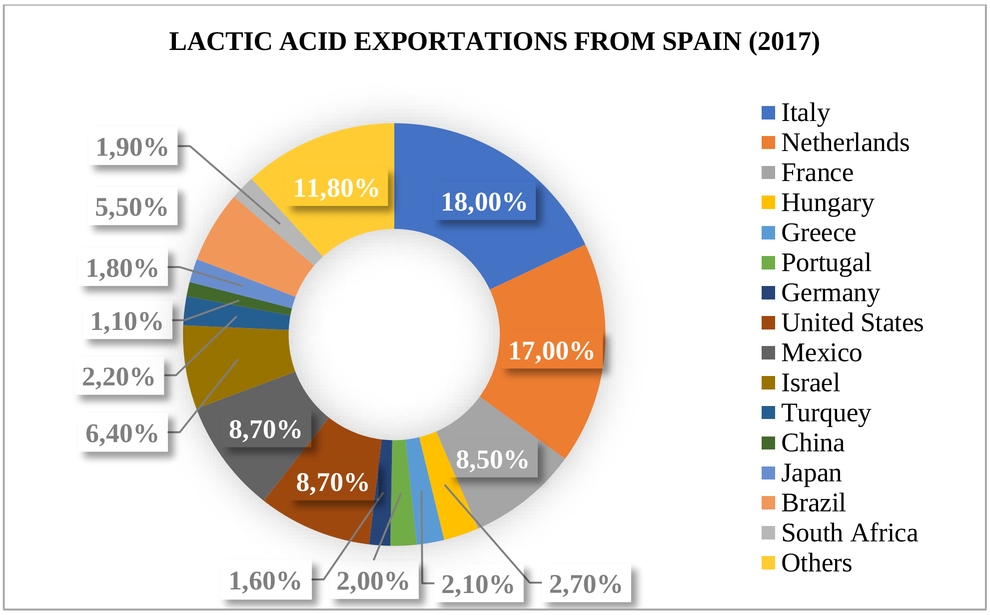


Figure 7. Lactic acid exportations in Spain, 2017. [3]

4.7.1.2 Importations

As explained above, Europe was the market region leading the market exportations. Analyzing importation data is proved that Europe is also the largest lactic acid importer region in the world. Europe exported lactic acid to a total value of US$ 275 million in 2017. As shown in figure 8, and comparing with figure 4, the largest exporters are, at the same time, the largest importers.

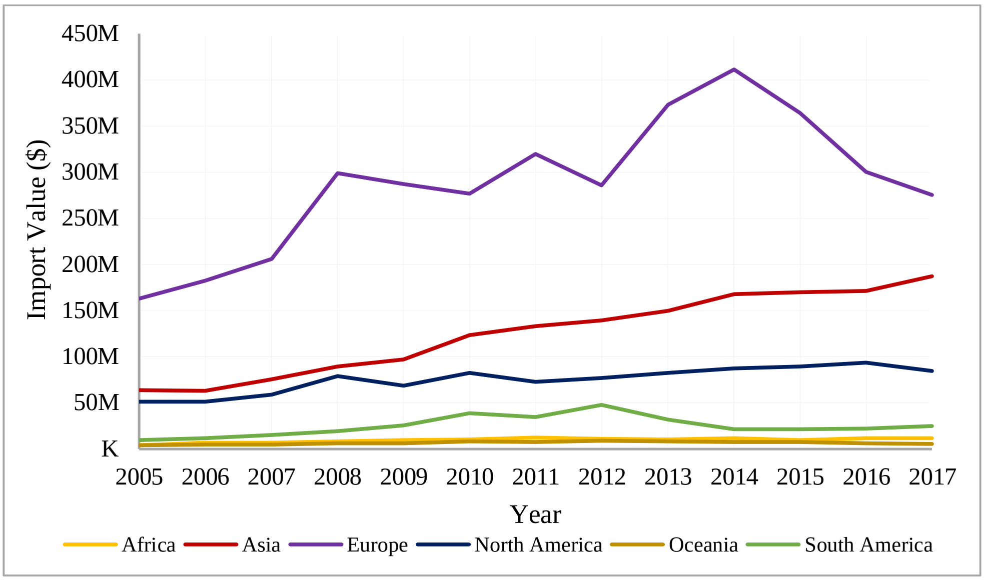


Figure 8. Lactic acid import trends around the world. [3]

Asia imported lactic acid to a total value of US$ 187 million and North America imports to a value of US$ 84.3 million. Taking into account these values, a trade balance between exportations and importations can be considered. This balance was positive in 2017 for Asia and Europe and was negative for the rest of the regions. A negative balance indicates that importations are higher than exportations.

In Europe, the largest lactic acid importers are Netherlands, Spain and Germany, as displayed bellow in figure 9. The previously named countries imported to values of US$ 46.5 million, US$ 46 million and US$ 44 million respectively in 2017. It was also noted that, just like shown for the global market, in 2014 the importation values were reduced.

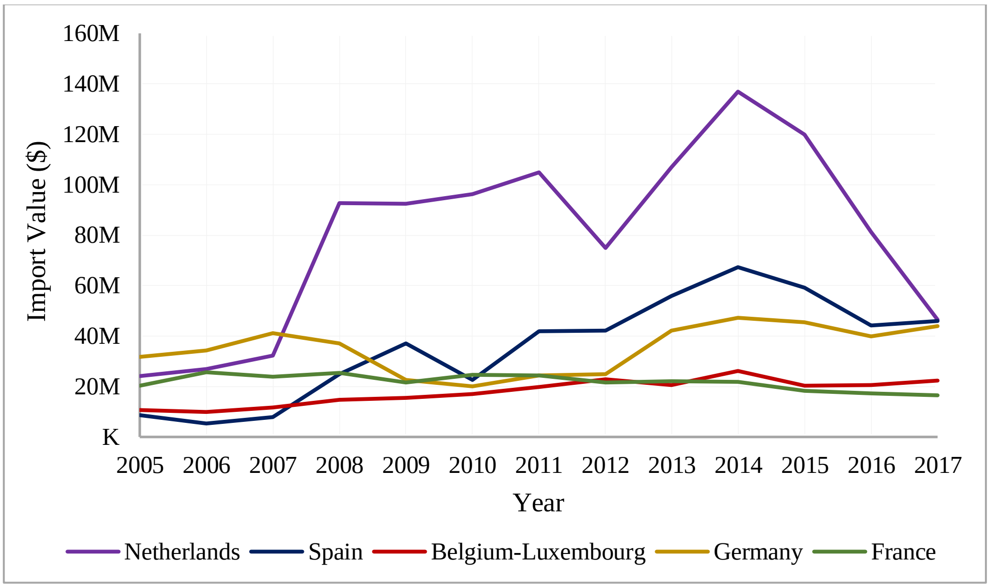


Figure 9. Lactic acid import trends for the main European import countries. [3]

In addition to the countries shown in the figure 9, there are many others which stand out in the lactic acid European importation market. Some of them are pointed in figure 10, in where is also shown some data, expressed in percentage, which tries to gives information about the relative importance of the importer countries in the total European importation values.

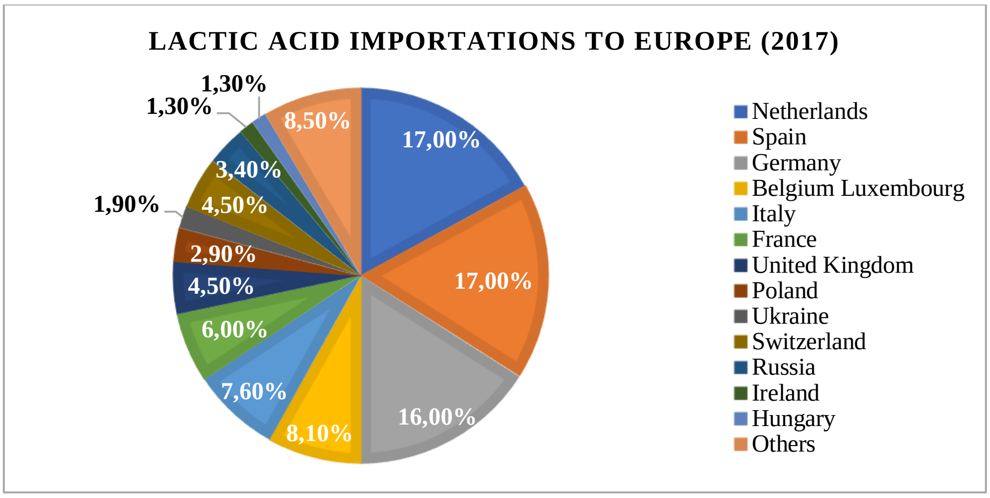


Figure 10. Lactic acid importations in Europe, 2017. [3]

In 2017, the importations carried out by Netherlands, Spain and Germany accounted for around 50% of the total importations made in Europe. In particular, Spain accounted for a 17% of these total importations.

The main share of the lactic acid Spanish imports come from Thailand, that is, the imports are coming from outside the European continent. Yet despite this, there are other significant countries such as Netherlands, Germany and France. Their relative importance in respect to the total national importation value are indicated in figure 11, so as information shown for any other countries.

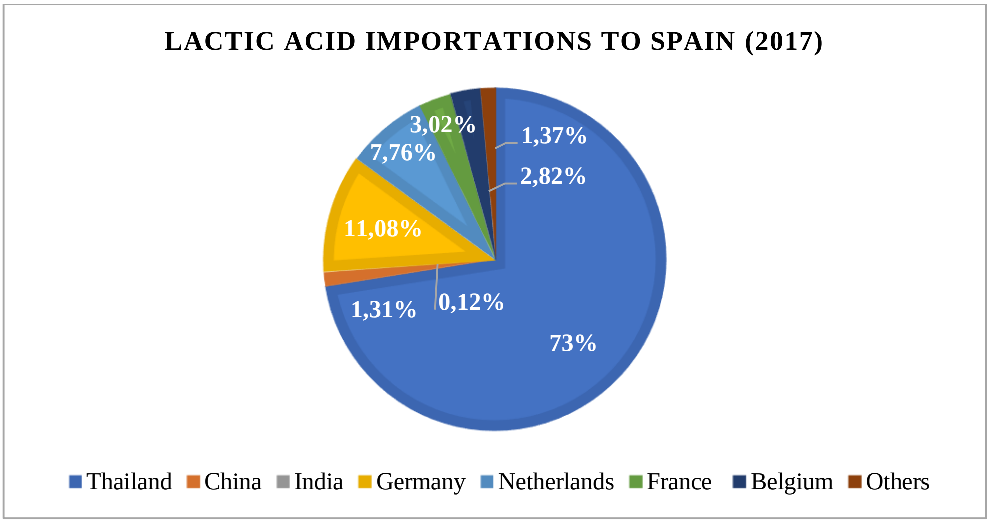


Figure 11. Lactic acid importations in Spain, 2017. [3]

In brief, the total Spanish importations can be said to be around a 74% accounting for the Asian region and a 26% coming from Europe, leaving the remaining 0.653% for importations accounting for the American continent.

4.7.2 Poly lactic acid (product)

4.7.2.1 Exportations

United States is the leading PLA producer and exporting country. In 2016, exportations were made to a total value of US$ 116.47 million. Another major exporting country is Netherlands with a value of US$ 41.82 million in exportations at the same year. In figure 12, some other countries are illustrated and is shown information of their PLA exporting value.

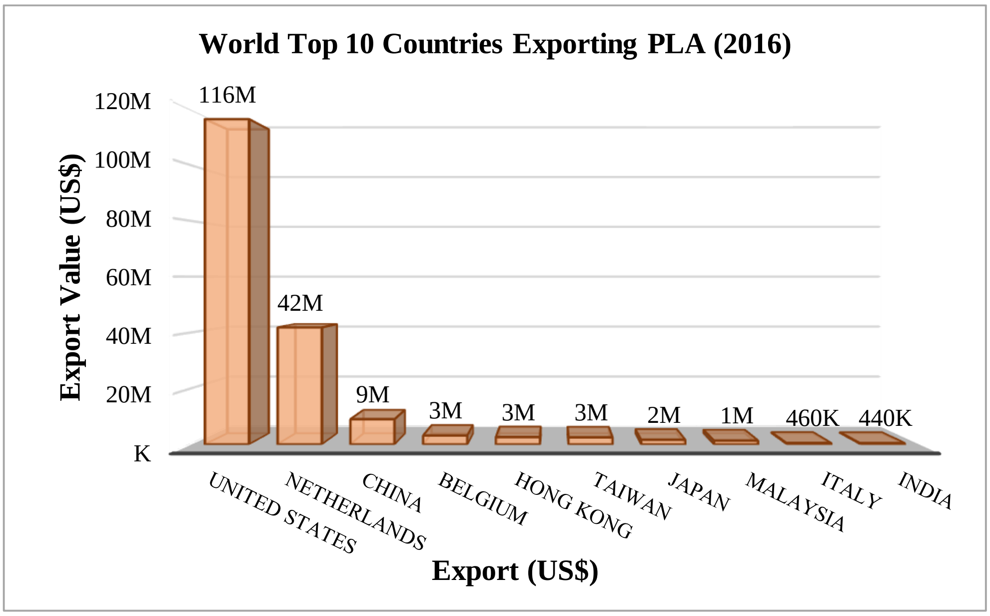


Figure 12. Mayor countries exporting PLA, 2016. [6]

The European Union have exported PLA to a value of 7.65 million € in 2017. Approximately a 60.23 % of the exports from European countries went to United States, although, as shown in the figure 13, Europe exports, to a lesser extent, to many other countries such as Taiwan or Russia.

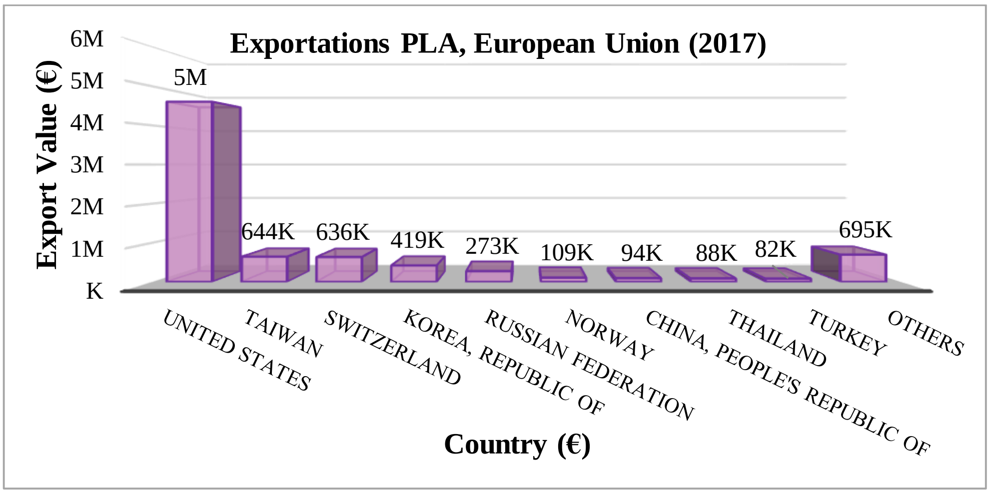


Figure 13. PLA exportations from the European Union, 2017. [10]

PLA Spanish exports remained inexistent until 2012, although in this year exports were very low. The highest export value was in 2015 and reach an approximate value of 287,000 €. The poly (lactic acid) exports dropped by 2,000 € in 2017 and has been exported to China, Serbia and Peru. In short, Spain has a very reduced PLA market.

4.7.2.2 Importations

Taiwan was the greatest PLA importer country in 2016. Importations were made to a total value of US$ 37 million. That same year, another major importing country is Netherlands with a value of US$ 32.8 million in the polymer importations. Since 2017, the demand is continuously increasing due to a favorable world legal context. In figure 13, some other countries are illustrated and is shown information of their PLA importing value.

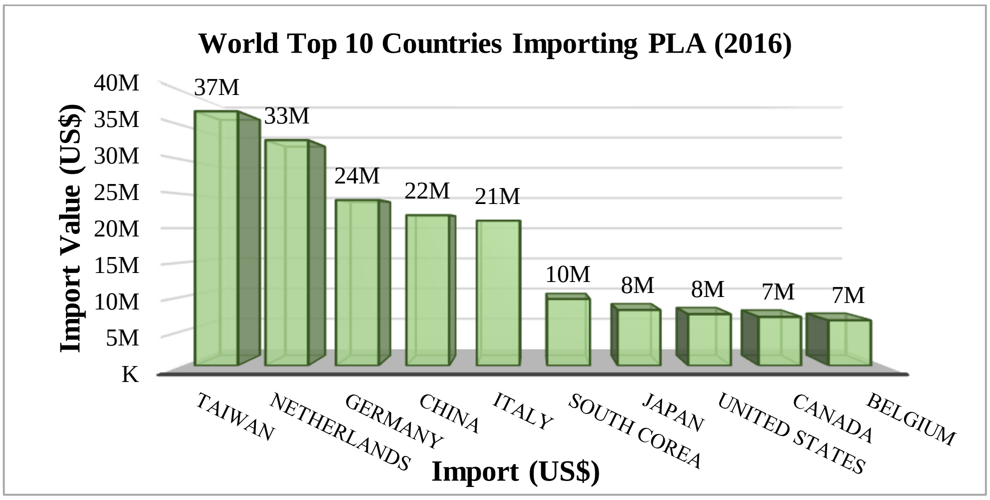


Figure 14. Mayor countries exporting PLA, 2016. [6]

The European Union have imported PLA to a total value of 58 million €. The value reach for 2017 was the highest recorded in this market and accordingly, the importations which have started in 2007 are showing a growth tendency. More data information about European importations are indicated in figure 15 and 17. As specified in figure 15, the European Union imports almost all the PLA from United States to a value of 51.56 million €, which represents an 88.76% of the total imports. Other countries from where the poly (lactic acid) is imported are: China, Korea, Japan, Israel, Switzerland, Thailand …

Spain started to import PLA from non-EU countries in 2007 with a non-stable biopolymer market. The demand increases and reduces ever since, but in 2017 the importations has risen to a value of 68,118 € from the value of 12,074 € reached in 2016. Spain has imported PLA from Switzerland, United States and China in 2017.

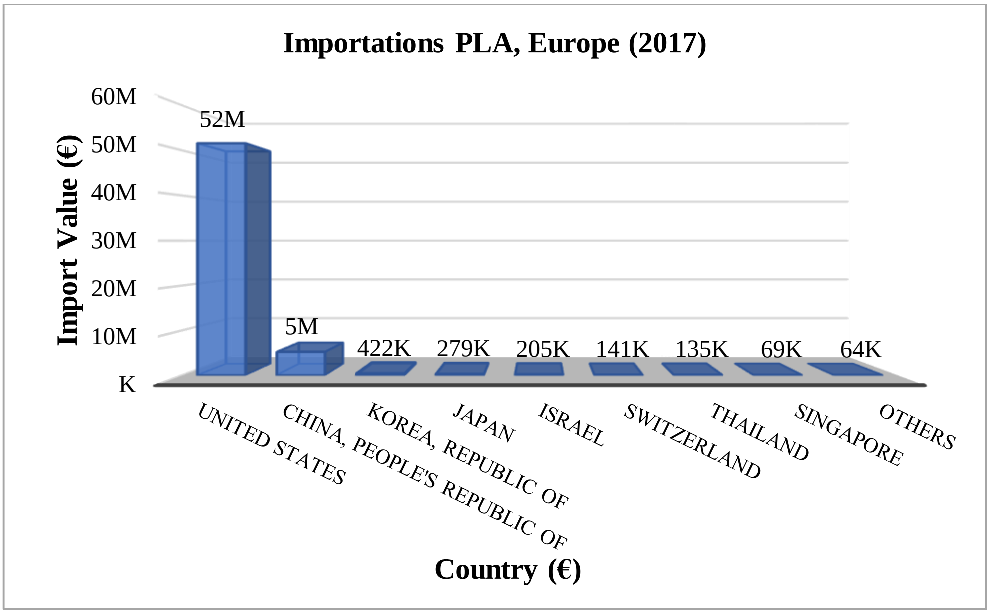


Figure 15. PLA importations in the European Union, 2017. [10]

4.7.2.3 Trade balance

Nowadays, the global trade balance of PLA is negative. Since 2011 this balance has been negative because the poly (lactic acid) imports have been greater than the exports. Figure 16 shows that PLA imports are valued in US$ 204.79 million in 2016, while the exports where valued in US$ 181.55 million. However, since 2014 the PLA exports are increasing and the imports are being reduced.

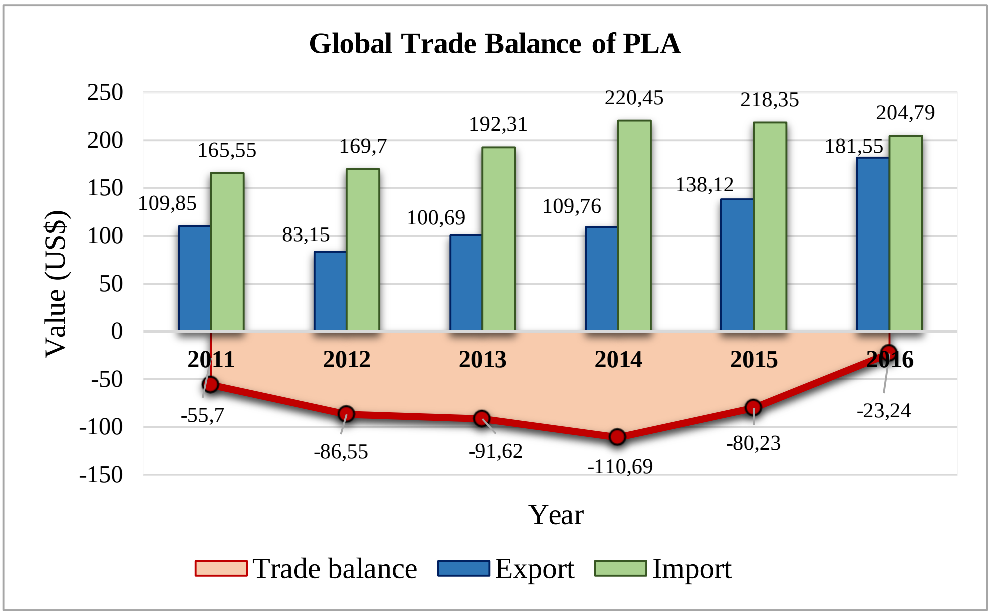


Figure 16. Poly (lactic acid) global trade balance. [6]

In Europe the global trade balance is also negative, but in this case the tendency balance (red line in figure 17) decreases every year since 2007. The imports are greater than the exports, accordingly to the previously explained in other sections of this project.

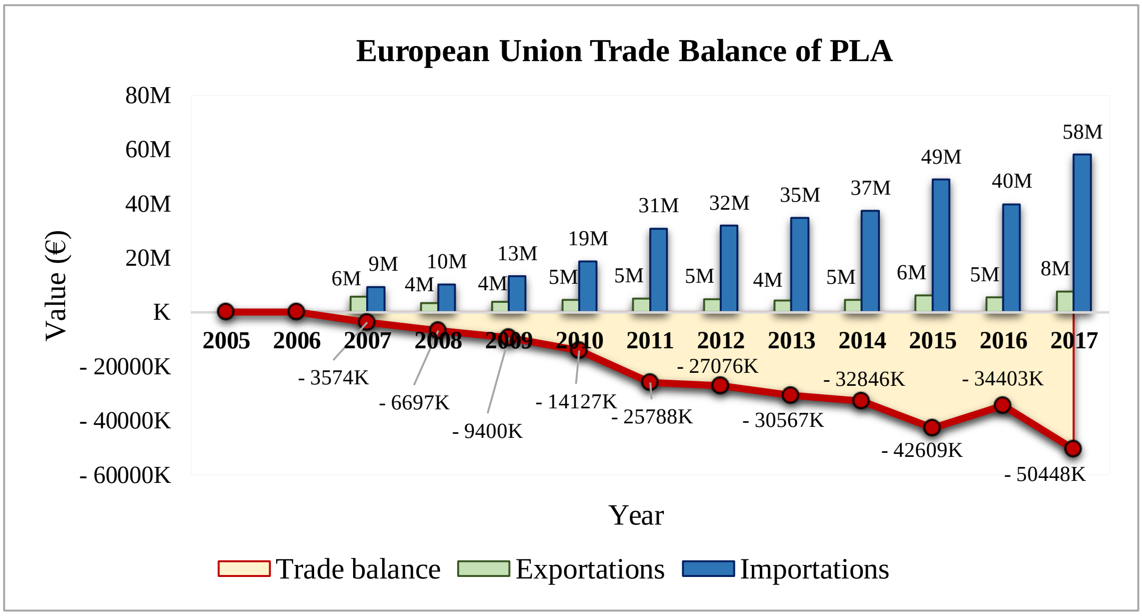


Figure 17. European Union Trade Balance of PLA. [10]

Spain has a very weak PLA market. The trade balance can be considered since 2007, and ever since a clear tendency is not shown. Must be taken into account that figure 17 and 18 are related to trade flows with EU and non-EU European countries.

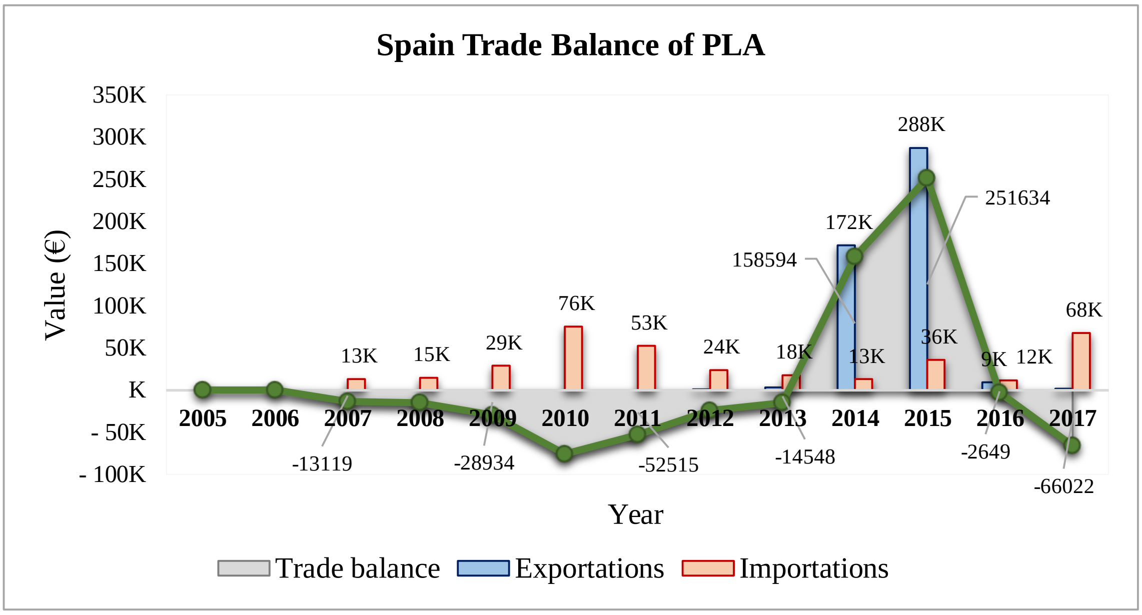


Figure 18. Spanish trade balance of PLA. [10]

4.8 Manufacturers and competitors

4.8.1 Raw materials manufacturers

The main lactic acid manufactures in the world are: The Dow Chemical Company, BASF S.E., Galactic S.A., Pyramid Bioplastics, NatureWorks LLC, Synbra Technology B.V., Corbion Purac, Danimer Scientific, Henan Jindan Lactic Acid Technology Co. Ltd, Wei Mon Industry Co. Ltd, Teijin Ltd, Musashino Chemical and Futerro.

In Spain there are many lactic acid manufacturers. Some of them are Lluch Essence S.L., ADITINSA Aditivos Industriales y Sabores S.L., HELM Ibérica S.A., PRINOVA S.L., INDUKERN S.A., PURAC Bioquímica S.A., EPSA Emilio Peña S.A., Barcelonesa de Drogas y Productos Químicos, S.A. and DIASA Industrial S.A., among others. [7]

4.8.2 PLA market competitors

Nowadays, there are a total of 25 enterprises with PLA production facilities seated in 30 different locations around the world. The total production capacity is 180,000 tons per year and the largest poly (lactic acid) producer (NatureWorks) is to be found in United States and Thailand. Its total production capacity is around 140,000 tons/year.

The major players in the poly (lactic acid) market are BASF SE, WeforYou, The DOW Chemical Company, Zhejiang Hisun Biomaterials Co., Corbion, TEIJIN LIMITED, Evonik, NatureWorks LLC, Synbra Technology bv, Danimer Scientific LLC, Galactic, Sulzer Ltd, Hitachi, Ltd., Musashino Chemical Laboratory, Ltd., Nantong Jiuding Biological Engineering Co., and others.

In Spain, some PLA market competitors are Viscofan S.A. and Condensia Quimica S.A. There are also PLA suppliers, such as Marsella Global S.L. This enterprise has reached to an agreement with PLANTURA Ltd. in order to supply 6,000 ton/year of PLA through the Iberian Peninsula.

4.9 Other information, consumables

The lactic acid is the main raw material of the project. However, that are other materials like catalyst and stabilizers that are being consumed during the operation of the facilities. Their price is important when determining the variable operation costs and is shown in table 1.

Table 1. Prices of the consumables. [11]

Consumable Item	Price (€/kg)
Stannous octoate	9.72
Trimethyl Phosphite	760.00
1-dodecanol	45.82
Phosphoric acid	1.77
2,6-di-t-butil-4-methyphenol	5.30

All these consumables will be renamed in this project for easier understanding: the stannous octoate will be known as catalyst 1, the trimethyl phosphite as stabilizer 1, a mixture of 1-dodecanol and stannous octoate as catalyst 2, the phosphoric acid as deactivating agent and the 2, 6-di-t-butil-4-methyphenol as stabilizer 2.

5. Raw materials

5.1 Lactic acid

5.1.1 Generalities

Lactic acid was discovered in 1780 by Carl Wilhelm Sheele who isolate it from sour milk and named it as “Mjölksyra”. This substance was first named as “acide lactique” by Lavoisier in 1789 and until 1857 was considered to be a milk compound. It was around this time when the lactic acid was first produced by fermentation. In 1881, the industrial production started in United States with a microbial process and in 1950 synthetic lactic acid was first synthetized in Japan. [12]

5.1.2 Properties

5.1.2.1 Physical properties

Lactic acid, also named as (2-hydroxypropanoic acid), is an enantiomeric molecule. It contains on its molecule structure a chiral carbon atom. Because of its chirality, the lactic acid can be named as L-lactic acid ((S)-lactic acid) and D-lactic acid ((R)-lactic acid). Each enantiomer differs from the other on its properties. Some physical properties of lactic acid, for both enantiomers and the racemic mixture, are shown in tables 2 and 3.

Table 2. Lactic acid physical properties. [12]

Property	Value
Formula	$C_3H_6O_3$
Molecular weight (g/mol)	90.08
Solid density (g/mL)	1.33 (solid, 20ºC)
Liquid density (g/mL, 20ºC)	1.224 (100% undercooled liquid) 1.186 (80.8% solution in water)
Solubility in water (wt.%)	86 (monomeric (S)-lactic acid, 20ºC)
Viscosity (mPa s)	28.5 (85.3% solution in water, 25ºC)
pKa (25ºC)	(S)- Lactic acid: 3.79 (R)- Lactic acid: 3.83 Lactic acid: 3.73 (racemic mixture)
Crystal structure	(S)- Lactic acid: orthorhombic, space group $P2_12_12_1$
Melting point (ºC)	(S)- Lactic acid: 53.0 (R)- Lactic acid: 52.8 Lactic acid: 16.8 (racemic mixture)

Table 3. Lactic acid physical properties (continuation). [12]

Property	Value
Boiling point (ºC)	122 (at 14 mmHg) (racemic mixture) 103 (at 14 mmHg) ((R-Lactic acid)) Aqueous solutions (120-130ºC range) 104ºC (at 6.5 kPa) (30% solution) 119ºC (at 6.5 kPa) (50% solution) 145ºC (at 6.5 kPa) (88% solution)
Specific heat (J/ (g K), 25 ºC)	Crystalline (S)- Lactic acid: 1.41 Liquid lactic acid: 2.34
Heat of fusion (kJ/mol)	(S)- Lactic acid: 16.8
Dissociation constant Ka (25ºC)	(R)- Lactic acid: 1.90×10^{-4} Lactic acid: 1.38×10^{-4} (racemic mixture)
Vapor pressure (mbar, 20ºC)	(S)- Lactic acid: 0.0041
Optical rotation in degrees	(S)- Lactic acid: +2.5 (R)- Lactic acid: -2.5

Besides the data shown in tables 2 and 3, other physical characteristics for lactic acid are known: It is a white crystalline powder and a colorless liquid and its melting point is low if compared with other polyesters like non-biodegradable polymers such as PET (polyethylene terephthalate) (254-256ºC). Moreover, it is an odorless nonvolatile acid which has a mild acidic taste.

5.1.2.2 Chemical and thermodynamic properties

The lactic acid molecule, as shown in figure 19, is a three-carbon compound with a -COOH group (acid functional group) and a -OH (hydroxyl group). Both groups may react with each other according to esterification reactions and linear dimers of lactic acid may be formed. From this dimer, lactide may be synthetized.

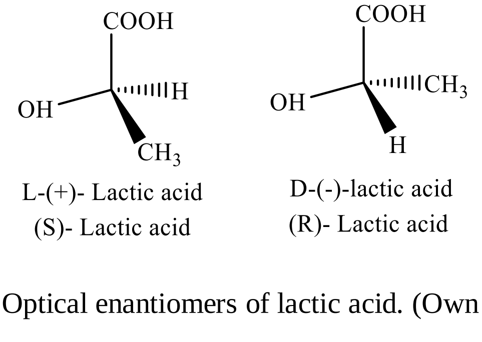


Figure 19. Optical enantiomers of lactic acid. (Own authorship)

Lactic acid is a moderate organic acid which dissociates in water resulting in ion lactate and H^+. Lactic acid dissociation is a reversible reaction but, when the pH is higher than the pKa, the lactic acid will dissociate to lactate, as indicates in figure 20.

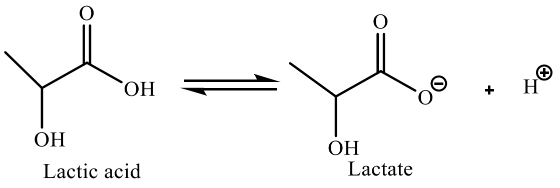


Figure 20. Dissociation reaction of lactic acid to lactate. (Own authorship)

The lactic acid can react with metals in order to produce hydrogen and metal salts. It forms dilactide by esterification with alcohols, glycol is produced by hydrolysis and lactate esters are formed by catalytic dehydration. Moreover, can react with hydrogen cyanide and diazo compounds and flammable or toxic gases are being released.

Table 4 summarizes thermodynamic parameters for lactic acid at 25ºC.

Table 4. Lactic acid thermodynamic parameter, 25 ºC. [12]

Thermodynamic Parameter	Crystalline L- (+)-Lactic acid	Racemic Lactic acid
Heat of dissociation (ΔH, cal/mol)	-63	-63
Heat of solution (ΔH, cal/mol)	+1868	-
Heat of fusion (ΔH, cal/mol)	+4030	+2710
Entropy of fusion (ΔS, cal/ (mol ºC)))	+12.2	+9.4
Heat of combustion (ΔH_c^o, cal/mol)	321,222	-325,600
Heat of formation (ΔH_f^o, cal/mol)	165,890	-163,000
Heat of capacity (Cp, cal/ (g ºC))	+0.338	+0.559
Entropy of formation (ΔS_f^o, cal/ (mol ºC)))	-137.2	-125.3
Free energy of formation (ΔF_f^o, cal/mol)	-124,980	-126,500

5.1.3 Lactic acid characteristics for the production process

The lactic acid purity is an essential parameter for the production of a high molecular weight poly (lactic acid). Nowadays, there are several industrial production processes for the manufacturing of this polymer with the desired purity. Despite this, some impurities from the fermentation growth of the lactic acid and further processing remain in solution and enters the process.

Table 5. Some lactic acid impurities. [13]

Impurity	
Lactates	Ethyl lactate, Methyl lactate and butyl lactate
Organic acids	Acetic acid, glyceric acid, succinic acid, formic acid, fumaric acid, pyruvic acid and oxalic acid.
Alcohols	Butanol, ethanol, methanol…
Amino acids	Alanine, glycerine, serine and glutamine
Other fermentation by-products	Metabolic intermediates, colour bodies, cell mass…

Some general lactic acid impurities are shown in table 5. Nevertheless, the commercial lactic acid is pretty pure and the following concentration impurities are commonly detected: chlorides and sulfates (<10 mg/L), iron and heavy metals (<5 mg/L), arsenic (<1 mg/L), alcohols like methanol, methyl ester…Moreover, a 97-98% purity of the commercial lactic acid is estimated. Lactic acid purity must be high because the lactic acid impurities amount must be lower than 0.05%mol previously to the high molecular with PLA polymerization step. High impurity involves a reduction in the PLA molecular weight. Impurities like butanol or butyl lactate act as catalyst in the polymerization reaction and degrade the polymer if they are not remover in previous steps. [13]

With this in mind, lactic acid 80%wt solution with a 95% L (+)-lactic acid esteroisomeric purity (as indicated in the safety sheet) is the feeding for the poly (lactic acid) production process. This process requires a feed raw material between 25%wt and 88%wt. Concentrations below 25%wt are not recommended because of the large energetic consumption and great wastes generation. Concentrations beyond 88%wt at normal conditions have a huge amount of oligomers due to oligomerization of the lactic acid at equilibrium. The amount of impurities in the lactic acid is considered to be 97%.

6. Products

6.1 Poly (lactic acid)

6.1.1 Generalities

The poly(lactic) acid or PLA is a biodegradable biopolymer. It is a renewable, stable, odorless, clear, shiny aliphatic polyester with similar characteristics to polyethylene terephthalate. PLA can be produced from lactic acid and, depending on the manufacturing process, can develop different mechanical properties. The lactic acid required as raw material can exist in three optically active configurations, or stereoisomers: L-lactic acid (LLA), D-lactic acid (DLA) and DL-lactic acid (DLLA). L-lactic acid can be produced by a biological (fermentation) or a chemical reaction pathway, however, the latter named stereoisomers can only be manufactured by the chemical reaction pathway.

There are several chain configurations and grades of PLA according to the corresponding acid lactic enantiomeric configuration monomers. The PLA stereochemistry has effects on the physical and mechanical properties, so for each chain configuration there will be differences and similitudes on the PLA properties. The PLA grades are: poly (L-lactic acid), poly (D-lactic acid) and poly (DL-lactic acid). Furthermore, the PLA stereochemistry is related to its molecular structure because the PLA constitutional unit contains an asymmetric carbon atom with a helical conformation. The molecular structure of a PLA unit is shown in figure 21.

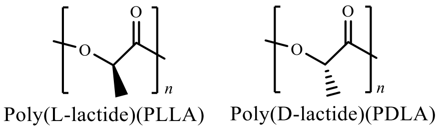


Figure 21. Molecular structure of PLA (stereochemistry).

The stereochemical structure of PLA have influence on the crystallinity, which is defined by the weight fraction of the corresponding PLA chain configuration in the manufactured polymer. The crystallinity have an impact over some other properties, such as the biodegradation of the material.

From this basis, the PLA can be semicrystalline or amorphous. PLLA is semicrystalline, while PDLLA is amorphous. The latter configuration polymer is amorphous because of the aleatory distribution of the L- and D- lactic acid units. By increasing the crystallinity, so as the degree of polymerization, some other properties like the strength, melt temperature, elastic modulus and glass transition temperature increases.

The crystallinity along with the molecular weight and the polymer composition are the basis for the specific physical, mechanical, biological and physiological properties of the polylactic acid.

Some general PLA properties are: high hydrophilicity, low heat resistance, low impact strength, high transparency, high resistance to scratch, high young´s modulus, high scalability, good printability and high biodegradability.

The biodegradability is related to the capacity of PLA to be transformed again into LA, just like indicates the equilibrium reaction between both materials. The microorganisms secrete enzymes to break into smaller fragments the PLA during continuous hydrolysis and oxidizing reactions.

6.1.2 Properties

6.1.2.1 Mechanical properties

The polylactic acid has different mechanical properties depending of the molecular weight and the stereochemistry of the lactic acid units from which the polymer is formed. This is the case of the tensile modulus and the strength of the PLA. The value of the tensile modulus is multiply by a factor of two when the molecular weigth increases from 50,000 to 100,000 g/mol and the strength increases from 15.5 to 150 MPa when M_w raises from 50,000 to 200,000 g/mol. The polylactic acid mechanical properties must be calculated for each particular case. Table 6 gives, as example, some information about the mechanical properties of a high molecular weigth PLA.

Table 6. Mechanical properties for high molecular weight PLA. [12].

Property	PLLA		PDLLA
Annealing at 105 ºC	No	Yes	-
Molecular weight (M_w, g/mol)	67000	71000	11400
T_m (ºC)	181	178	-
Crystallinity (%)	3	45	-
Tensile properties			
Yield strength (MPa)	70	70	53
Tensile strength (MPa)	59	66	44
Yield elongation (%)	2.2	2.0	1.5
Elongation at break (%)	7.0	4.0	5.4
Elastic modulus (MPa)	3750	4150	3900
Flexural properties			
Flexural strength (MPa)	106	119	88
Maximum strain (%)	4.7	4.6	4.2
Elastic modulus (MPa)	3650	4150	3600
Impact resistance			
Izod, notched (kJ/m^2)	2.6	6.6	1.8
Izod, unnotched (kJ/m^2)	19.5	35.0	15
Heat resistance			
HDT (ºC)	55	61	50
Vicat penetration (ºC)	59	165	52
Hardness			
Rockwell hardness (scale H)	88	88	76

6.1.2.2 Thermal properties

The polylactic acid is a thermally stable polymer at room temperature, however, starts its breakdown in the range of temperatures 230-260ºC and, in presence of water or other aqueous solutions can start hydrolysis reactions and other side reactions without catalyst at 200ºC.

The thermal properties, just like the mechanical properties, are very affected by the stereoisomery. Some of them are the glass transition and melting temperatures and the enthalpies of melting and crystallization.

The melting point of the polymer varies with the crystallinity, optical purity and the molecular weight. The pure L-type polymer is semicrystalline with a crystallinity above 70% and has a melting range over 180ºC with an enthalpy of melting of 40-50 J/g. However, for non-pure PLA the typical values of the melting point are ranged around 130-160ºC.

The glass transition temperature is approximately 45ºC for low molecular weight although sharply increases when the molecular weight rises. The crystallization temperatutes are in a range of 110-130ºC and increases with the molecular weight. The heat of crystallization, however, does not increase with the molecular weight.

Some thermal properties are shown in table 7. The molecular weight and the stereoisomery are the two aspects to take into account when comparing the values of the properties.

Table 7. Thermal properties of PLA for different isomer types and molecular weights. [12]

Isomer type	**M_n x 10^3 (g/mol)**	**M_w/M_n**	**T_g (ºC)**	**T_m (ºC)**	**ΔH_m (J/g)**	**T_c (ºC)**	**ΔH_c (J/g)**
PLLA	4.7	1.09	45.6	157.8	55.5	98.3	47.8
	7.0	1.09	67.9	159.9	58.8	108.3	48.3
	14.0	1.12	66.8	173.3	61.0	110.3	48.1
	16.8	1.32	58.6	173.4	61.4	105.0	38.1
PDLA	13.8	1.19	65,7	170.3	67.0	107.6	52.4
	16.5	1.2	69.1	173.5	64.6	109.0	51.6
PDLLA	4.3	1.90	44.7	-	-	-	-
	7.3	1.16	44.1	-	-	-	-

M_n = Molecular number; M_w = Molecular weight; T_g = Glass transition temperature; T_m = Melting temperature; Tc = Enthalpy and crystallization temperature; ΔH_c = Enthalpy of crystallization; ΔH_m = Enthalpy of melting.

A summary of the thermal conductivity of the polylactic acid is shown in figure 22. The thermal conductivity increases until 90ºC, temperature at which this property stabilizes. The thermal conductivity is a significant property for the polymer because of its great influence during the heat removal in polymerization reactions.

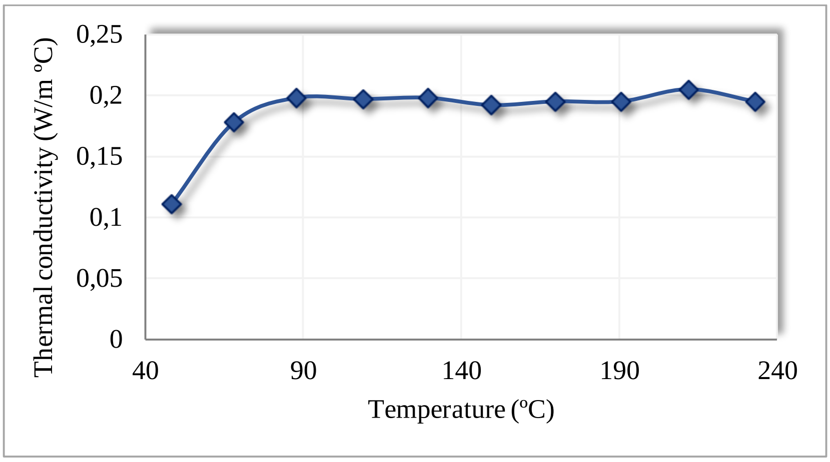


Figure 22. Thermal conductivity behavior of the polylactic acid. [12]

Finally, the heat capacity of the polylactic acid can be estimated in J/mol K from equations 1 and 2.

$$C_{p,liquid} = 120.17 + 0.1706\ T\ (K) \tag{1}$$

$$C_{p,solid} = 25.153 + 0.2302\ T\ (K) \tag{2}$$

6.1.2.3 Other physical properties

The poly (lactic acid) can be described with the physical properties shown in table 23.

Figure 23. Other physical properties of the polylactic acid. (Own authorship)

Property	Value
Chemical formula	$(C_3H_4O_2)_n$
Physical state (25°C)	Solid
Ignition temperature	388°C
Color	Various
Smell	Slight
Glass transition	60-65°C
Melting temperature	130-160 °C
Printing temperature	178-240°C
Injection molding temperature	170-200°C
Extrusion molding temperature	180-240°C
Lamination temperature	200-240°C
Spinning temperature	180-240°C
Inflation molding temperature	170-190°C
Density	1.21-1.43 g/cm^3
Tensile strength	49-56 MPa
Tensile elongation	0.5-9.2%
Flexural strength	48-110 MPa

Nevertheless, the solubility of poly (lactic acid) must also to be considered. This biopolymer, just like other lactic acid-based polymers, is not soluble in hydrophilic solvents such as water, methanol, ethanol and unsubstituted hydrocarbons, but is soluble in chlororoform, tetrahydrofuran, acetone, dioxane, hot benzene and methylene chloride when is heated. The poly (lactic acid) solubility is strongly dependent on the crystallinity. The interchain migration for the structures of the solvent is hindered by a high orientation of the polymer molecule. The crystallinity increases the free energy of mixing. Therefore, and in agreement with thermodynamic laws, when this free energy is positive the solubility is not possible.

6.1.3 Applications

PLA is a thermoplastic biopolymer with applications in very diverse areas, such as the textile industry, medical and pharmaceutical industry, agriculture and environment issues, food industry… This polymer can be seen as a competitor of the petrochemically-based plastics due to its wide properties range. This is mainly due to PLA properties changes according to its crystalline state, polymer molecular weight and the fraction of stereoisomers D- and L-, so as the copolymerization, in the final manufactured polymer. Some applications are explained in detail in the next sections of this project.

6.1.3.1 Textile industry

For fiber applications, PLA polymers have properties similar to PET (polyethylene terephthalate), although PLA exhibit lower densities, lower refractive index, higher hydrophilic behavior and higher bending and stretching strengths. Moreover, PLA polymers have other properties which makes them suitable for this kind of applications: little discoloration of fabrics, bacteriostatic, weathering resistance, low smoke material, flame-retardant and low degree of shrinkage. [14]

The following are some textile applications of the polylactic acid:

- **Industrial fabrics**: Polylactic acid fibers can be applied, for example, in the automobile sector by using woven and nonwoven fabrics in seat cushions, door trims, ceiling fabrics, …
- **Filters:** PLA is a nontoxic polymer and use to have applications in where there is direct contact with food. PLA fibers have applications for food filters (such as tea and coffee filters), although have also air filter applications having antibacterial effects.

- **Towel and wipes:** Towels of PLA materials have faster drying, low shrinkage after being used and do not generate bad smells because of the antibacterial effects. PLA can also be applied in wipes for baby care or in other personal cares.
- **Home furnishings:** Some PLA properties such as UV stability, low flammability, antibacterial effects, stain resistance… includes PLA as an ideal material to the manufacturing of home and office furniture such as curtains, pillows, sheets, blankets, …
- **Clothing:** PLA fabrics has application for garments such as underwear, jeans, jackets, …

6.1.3.2 Medical and pharmaceutical industry

PLA is a biopolymer which fulfills some medical requirements for its application inside the human body. These requirements include nontoxicity, effectiveness, sterilizability and biocompatibility. As PLA is biodegradable, do not require long-term biocompatibility and may not produce immune rejections. Although biodegradable polymers may satisfy these requirements, they are not widespread use in medical applications because the degradation rate when the polymer is inside the human body must be the same is the rate for tissue regeneration and the biopolymer, when degrading, may decompose into toxic compounds. However, PLA do not have toxic effects during its degradation because during the hydrolytic reaction the polylactic acid becomes into lactic acid monomers, which are converted in the body into pyruvic acid to finally yield to carbon dioxide and water. [14]

The following are some general pharmaceutical applications of the polylactic acid: biodegradable scaffolds for tissue engineering implants, fibers, meshes, surgery material, bone fixation devices, preparation of biodegradable microspheres, microcapsules and thin coatings; antiviral administration, etc. Some of the most important are:

- **Fibers:** For absorbable sutures and for cardiovascular or urological surgeries in form of stents.
- **Meshes:** Creation of 3D structures for bone reconstruction and skin or cardiovascular structures regeneration among others.
- **Bone fixation devices:** Plates, pins, screws and wires of biodegradable material as PLA eliminates secondary surgeries to remove these fixation devises, eliminates other diseases caused by implants, also eliminates corrosion of implants made of metallic materials and avoid interference with other medical treatments.

- **Microspheres, microcapsules and thin coatings:** Microspheres are used in facial regenerating surgery. Microcapsules are applied for drug production because the drug release happens slowly. [14]

6.1.3.3 Food industry

Some short life basic products for human consumption can be transported and storage in containers of packages made of biodegradable polymers, such as PLA. Although this is one of the most spread and known applications for PLA polymers, food packaging cannot be used for all products. PLA has a high affinity to water and potential for fungal growth, both negative for some uses. [14]

6.1.3.4 Agriculture and environment

Nowadays, the agricultural activities are producing a large amount of plastic wastes. Most of them are resistant to degradation in short-term and are accumulating giving rise to problems related to their disposal. Against this background, the discovery of new polymers with degradable capacity, such as PLA, implies a reduction in the environmental impact.

In addition to this environmental impact reduction in agricultural lands, PLA can be used for bioremediation of soils, land surfaces and groundwaters. This is happening because PLA in aqueous phase acts as electron donor to the environment, according to an anaerobic process. Additionally, PLA can be a substrate source for damage lands. PLA polymers can release lactic acid monomers according to a hydrolysis reaction which performs slowly over the time. [14]

7. Study of alternatives

7.1 Reaction pathway study

PLA is one of the most extensively research and utilized biopolymer. PLA was first synthetized in 1932 by Carothers (at Dupont) and, ever since, different ways to synthetize it have emerged. Although at Dupont, initially, the PLA was only produced with low molecular weight, nowadays, high molecular PLA is expected to be fabricated. The PLA synthesis requires for all reaction pathways a strict control of the process conditions, which is the reason why none of them are easy to execute. There are two major routes for the PLA synthesis based on the lactic acid polymerization: polycondensation and ring opening polymerization. Polycondensation, simultaneously, includes methods like direct condensation, solid-state polycondensation and azeotropic dehydration. [12]

7.1.1 Lactic acid-based polymers by polycondensation

PLA can be produced from the lactic acid polymerization because, lactic acid, also named as 2-hydroxy propionic acid, has both -OH and -COOH groups. The hydroxyl and carboxylic acid groups react directly with each other to produce water and polylactic acid. The water needs to be removed as long as the equilibrium reaction takes place because the reaction needs to be shift to the right, LA to produce PLA.

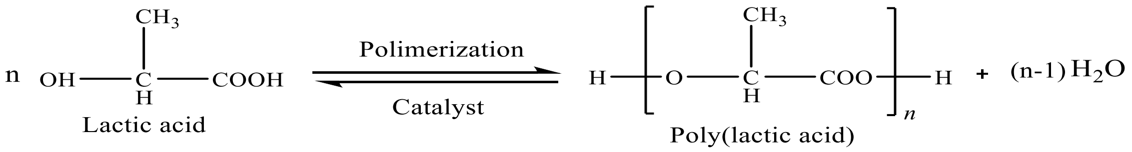


Figure 24. Condensation reaction for PLA production. [12]

Moreover, the more water is removed the better the reactive process selectivity. With better selectivity, side reactions, like transesterification reactions, can be avoided as much as possible. It is imperative that the polycondensation reaction should be the main reaction. According to all of this, the water removal should be enhanced in order to prevent the negative impacts of the side reactions on the polymer properties. Side reactions contributes to the formation of ring structures, which used to lower unwillingly the molecular weight of the polymer. One typical ring structure molecule form when this reaction system is carried out is the lactide, whose production rate becomes important with temperatures higher than 200ºC. Low temperatures have positive effects on the lactide suppression, however, the reaction rate is lower too because of a reduction on water removal by evaporation.

7.1.1.1 Direct condensation

Direct condensation polymerization is divided into three main steps: free water removal, oligomer polycondensation and melt polycondensation. It is considered to be one of the cheapest process for PLA production although has difficulties to specified the molecular weight to be achieved during the fabrication process because of complications on water removal.

- **Step 1- Free water removal:** The free water can be removed by a thermal phenomenon such as evaporation, using equipment known as evaporators. The main objective is to eliminate the excess of water capable of facilitate the formation of oligomers of lactic acid.
- **Step 2- Oligomers polycondensation:** Conversion of the lactic acid into low molecular weight PLA. The polycondensation can conduct in a stirred reactor or in an evaporator and the reaction rate for this conversion basically depends on the catalyzer to be used. The catalysts can be strong acids or organometallic compounds.
- **Step 3- Melt polycondensation:** On this step becomes important and efficient water removal while the water is being produced on the polycondensation reaction. An efficient water removal can be made by driving the reaction under low pressures, inert conditions and in a well-mixed system. In contrast to the oligomers condensation step, the reaction rate depends on the mass transfer of the water.

7.1.1.2 Solid-State polycondensation

In the solid state polycondensation there are four steps: the three first steps which were previously described in direct polycondensation, and a new last step or fourth step. The main goal for the introduction in the process of this new step is the obtention of a higher molecular weight PLA.

During this step, melt-polycondensated PLA is cooled until a temperature below its melting point. As the temperature descends and the polymer solidifies there are particles in continuous formation, a crystallization process takes place. The crystallization has two phases: crystalline and amorphous. In the latter are concentrated the catalyst and the reactive groups, which indicates that the polycondensation reaction performs at low temperature in solid state. The rate of the reaction depends on the mass transport of the water obtained in the reaction and, as happened in the melt polycondensation step (step 3), the water removal improves by driving the reaction under low pressures and inert conditions. [12]

7.1.1.3 Azeotropic dehydration

There are several patent applications for the production of high molecular weight PLA with azeotropic dehydration. All of them have a similar procedure if compared to the aforementioned methods, but the polycondensation proceeds in solution and the polymer obtained is collected with organic solvents. This method allows for a higher PLA purity but is also a higher time-consuming method with a very restricted temperature condition. Moreover, this technique requires various diacids, diols, hydroxyl acids and sophisticated catalyzers which remains as impurities, which is a clear disadvantage.

The water or solvent produced during the reaction performing is removed relatively easy by azeotropic dehydration using molecular sieves as drying agent. [12]

7.1.2 Lactic acid-based polymer by ring-opening polymerization

The ring opening polymerization (ROP) is a solvent free process which produces polylactic acid with the desired molecular weight. The process has three stages carried out in the following order: polycondensation, lactide manufacturing and ring-opening polymerization. In figure 25 are shown the three stages to perform the reaction route for the ROP process.

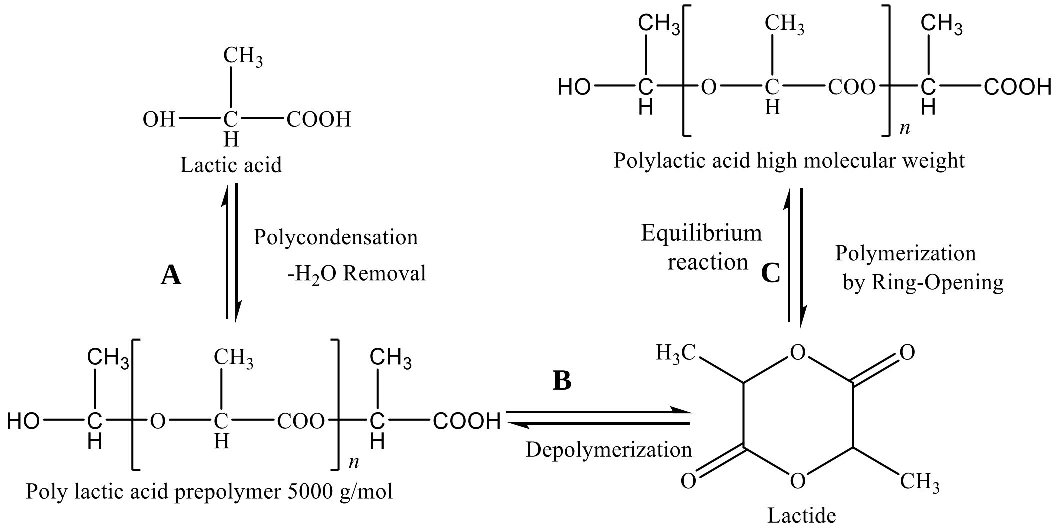


Figure 25. ROP process: A) Polycondensation, B) Lactide manufacturing and C) Ring-opening polymerization. (Own authorship)

The ROP is characterized by some important parameters: racemization, lactide purity and residual monomer content. The racemization can be defined as a conversion in where an enantiomerically pure mixture is turn into a mixture with more than one enantiomer (for example a mixture with D and L enantiomers). The racemization is directly dependent on the optical purity of the lactic acid from where PLA is produced. This phenomenon affects to the specific properties of the PLA as final product. For example, poly (D-lactide) acid (PDLA) and poly (L-lactide) acid are semi crystalline biopolymers, but the racemic mixture, named as poly (DL-lactic) (PDLLA), is an amorphous polymer. As regards the lactide purity, impurities (oligomers, acids…) might affect the final molecular weight or the polymerization rate. Moreover, the lactide must be removed from the polymer-end product because changes in the properties of the material and negative effects during the final processing of the polymer can be produced. [12]

- **Polycondensation:** In the ROP process the polycondensation is the first stage to be carried out and has many patents, such as the Cargill process, the Inventa Fisher process and the Boehringer process. Each patent has its own characteristics: different catalyzer systems, temperature increase conditions (105-150ºC) and pressure decrease conditions (350-30 mmHg). During this stage, low molecular weight (preferably 400-2500 g/mol) PLA, named as prepolymer, is being manufactured from lactic acid.
- **Lactide manufacturing:** The lactide (cyclic dimer) is obtained from the PLA prepolymer manufactured in the early stage by an equilibrium reaction. According to the equilibrium, the temperature and the pressure are manipulated and the lactide is produced. However, the lactide will contain impurities such as water, lactic acid, oligomers, lactoyllactic acid, lactoyllactoyllactic acid and meso-lactide and a purification is needed before the next stage can proceed. The purification can be made according to these approaches: solvent assisted purification, crystallization from the melt and distillation.
- **Ring-opening polymerization**: This stage is conducted by the ring-opening polymerization reaction for the preparation of high molecular weight PLA from lactide. The lactide polymerization can be performed with melt polymerization, bulk polymerization, solution polymerization and suspension polymerization. Furthermore, there are 3 reaction mechanisms in this reaction route: cationic, anionic and coordination mechanisms. Both, anionic and cationic polymerization becomes a cause of undesirable side reactions. The cationic ring-opening polymerization is achieved using Lewis and protic acids and, alkylating and acylating agents while for the anionic ring opening polymerization strong nucleophilic or bases are required. The coordination mechanisms employ a wide variety of initiators and catalysts which acts as a Lewis-acidic metal center for the corresponding monomers. [12]

7.2 Justification of the selected alternative

Various reaction routes have been studied for the poly (lactic acid) production from lactic acid. The reaction route selection made in this project has taken into account several aspects like: the process economy and the product value, energy exploitation and recovery, process safety, environmental compatibility, technical viability for the industrial process, operation conditions and product requirements.

Direct polycondensation is conducted at vacuum pressure and high temperature conditions without catalyzer. The obtained polymer has low molecular weight due to the difficulty of the water removal, in special when the mixture of reactants and product increases in viscosity. The PLA characteristics depend on the molecular weight and the final product purity, among other aspects. Thus, changing the PLA characteristics the polymer prices increases and also the number of possible applications. Nowadays, direct polycondensation is the cheapest reaction route for the commercial process, however, it is not the most commonly used. The stereoisomery cannot be controlled with this process and hence a specific stereoisomer cannot be produced.

The rest of the reaction routes also require vacuum pressures and high temperatures for their performance. Solid-state polycondensation produces a low molecular weight PLA which has higher molecular weight than the one manufactured by direct polycondensation. The operating temperatures are lower for this route, if compared to other PLA manufacturing routes. However, the reaction rate is also lower and is more time-consuming.

Azeotropic dehydration polymerization produces a high molecular weight PLA. Nevertheless, solvents such as the diphenyl ether are required, as well as several reactors. Both reasons make the process control more complex.

The PLA manufactured with this reaction route will be very expensive and might become in a product with little market competitivity. Besides, the solvent is particularly tricky to eliminate from the final product. Accordingly, this is the less attractive process from an economical and environmental point of view.

The ring opening polymerization reaction route has the most currently used production process. A high molecular weight and purity product which is highly esteemed in the market is obtained. The process has a very high performance with a minimal waste's generation and a maximum raw materials utilization. It can be regulated in order to manufacture the product with the desired stereochemistry. A catalyzer is required.

The reaction routes and factors to be considered in the process selection are shown in table 8. The most and less favorable reaction routes will be indicated for each factor. A clear allocation cannot be made in some cases and will be chosen more than one reaction route alternative for the studied factor.

Table 8. Evaluation criteria for possible reaction routes. (Own authorship)

Evaluation criteria	Polycondensation			Ring Opening Polymerization
	Direct polycondensation	Solid-State polycondensation	Azeotropic dehydration	
Economic	✓	-	x	✓
Energetic	-	x	x	✓
Process Safety	✓	-	x	✓
Environmentally-friendly	✓	-	x	✓
Technical viability	✓	✓	✓	✓
Operation conditions and requirements	x	-	-	✓

✓ : Most favorable reaction route according to the evaluation criteria.

x : Less favorable reaction route according to the evaluation criteria.

The chosen reaction route is the ring opening polymerization. The main reason for this route selection is its process capacity to manufacture the desired product with a high purity: L-poly (lactic acid). The process performance is technically viable and there are several equipment and technologies available. It is not the cheapest process but produced a high-quality PLA with the demanded characteristics (with high price) and also allows for the energetic recovery in the reactors, which are at high temperatures.

8. Analysis of technical feasibility

The technical feasibility study provides information about the technology available for the conduction of the production process and the facilities construction. It is a procedure for the validation of the technology assumed and the design of the project. The viability considers:

- Development risk: Including the process and equipment security, the facilities control and the environment protection. Legal and political reasons are also incorporated in this study.
- Resources availability: Raw materials, catalyzers, utilities, labor force, etc.

- Technology: The production process availability, the fulfillment with current legislation of the equipment purchased and the used of updated technology.

8.1 Design Factors

8.1.1 Production process availability

The production process viability is linked to several factors. Some of them are related to the existence of equipment and raw materials for its development and many others are related to socio-economic aspects. An unprofitable process, both technologically and economically, must not be carried out. A certain product manufacturing is performed with a production process which is developed from the laboratory phase to the industrial phase and performing pilot producing scale verifications. Some of these processes are new inventions of private companies and are restricted under patents. In table 8 are shown some patents for the poly (lactic acid) production process. Despite patents are limiting the use of the process/invention to its beneficiary, they are providing examples about the current existence of industrial processes for the poly (lactic acid) manufacturing. It is also present in table 9 the name of some current poly (lactic acid) manufacturers.

Table 9. Several patents for the poly (lactic acid) production process. (Own authorship)

Patent number	Patent name	Assignation
US005142023A	Continuous Process for Manufacture of Lactide Polymers with Controlled Optical Purity	Cargill, Incorporated
US006326458B1	Continuous Process for the Manufacture of Lactide and Lactide Polymers	Cargill, Incorporated
US005357035A	Continuous Process for Manufacture of Lactide Polymers with Purification by Distillation	Cargill, Incorporated
US005508378A	Method for Producing Polylactic Acid	Shimadzu Corporation
EP2607399A1	Process for Producing Polylactic Acid and Reactors for Used in Said Process	Companhia Refinadora da Amazônia
US005470944A	Production of High Molecular Weight Polylactic Acid	ARCH Development Corpotation
US008674065B2	Methods for Producing Lactide with recycle of Meso-Lactide	NatureWorks LLC
WO01/38284 A1	Improved lactic acid processing; Methods; Arrangements; And, Products	Cargill Dow LLC
WO2010/012770 A1	Process for the Continuous Production of Polyesters	Rac Biochem BV and Sulzer Chemtech Ag

Table 10. Several patents for the poly (lactic acid) production process (Continuation). (Own authorship)

Patent number	Patent name	Assignation
US005574129A	Process for Producing Lactic Acid Polymers and a Process for the Direct Production of Shaped Articles from Lactic Acid Polymers.	The Japan Steel Works Ltd.
US008053584	Purification Process for Lactide	Tate & Lyle Public Limited Company
CA2732419C	Process for the Continuous Production of Polystesters	Purac Biochem BV and Sulzer Chemtech AG
US20120101248A1	Method for Producing Polylactic Acid	-
E10789463	Procedimiento para Producir Ácido Poliláctico	Toyo Engineering Corporation and Mushashino Chemical Laboratory Ltd.

8.1.2 Installation security

The polylactic acid production process operates with temperatures below 150ºC, which is lower than the critical temperatures of 400ºC. However, this process requires of vacuum pressures in other to enhance vapour liquid equilibrium, to avoid the degradation of the materials sensible to temperature, to allow liquid state of high boiling temperature substances, ... The operation is out of the security range of 1-10 bar. Nevertheless some security devices can be installed in the equipment such as relief valves and rupture disc or appropriate design of the equipment (design for full vacuum conditions)

The corrosivity of the lactic acid must also be taking into account for security. Corrosion allowances can be considered in pipelines and equipment.

8.2 Process factors

8.2.1 Raw materials availability

The lactic acid is currently available in the market. Spain is the second most important importer and exporter country of lactic acid in Europe. For this reason, an easy access to the raw material is assured. More specific information is provided in sections 4.8.1 and 9.2 of this project. In the first case are named some suppliers for Spain and the world and in the second case are highlighted some companies providing lactic acid near the plant location.

8.2.2 Technology availability

This section of the poly (lactic acid) production facility project focuses on the identification of the availability of the main process equipment. The recognition of the technology has been made and some suppliers for such technology were identified.

A pre-treatment of the raw materials (lactic acid) occurs in the section 100 of the production facility of poly (lactic acid). An evaporator operating at vacuum pressures is required for such action. Accordingly, there are different types of evaporators: rising film evaporators, forced film evaporators, falling film evaporators, natural circulation evaporators, etc. The selection of one them depends on the specifications shown in table 11.

Table 11. Different evaporator's characteristics. [15]

		Natural Circulation Evaporator	**Forced circulation Evaporator**	**Rising Film Evaporator**	**Falling Film Evaporator**
Evaporator-properties	Residence time	long	long	medium	short
	Pressure drop	medium	medium	medium	low
	Hydraulic head	high	high	medium	none
	Liquid hold-up	high	high	medium	low
	Product recirculation	by density difference	by pump	none	by pump
	Liquid velocity	Low/medium	high	Low/medium	medium
	Product film	Filled tubes, 2-phases	Filled tubes	Filled tubes, 2-phases	Thin, by gravity
	Heating temperature difference	Medium	Small	Medium/large	Small
Product-properties	Sensitivity to heat	Low fairly suited	Low/medium fairly suited	Medium fairly suited	Medium suited
	Fouling	Vulnerable	Little	Little/medium	Vulnerable
	Solids presence	Suited	Well suited	Fairly suited	Fairly suited
	Foaming	Fairly suited	Fairly suited	Suited	Suited

The reasons of the selection of one of these evaporators are explained in the section 11.1.2 of Document I. Descriptive report. Many of these evaporators are currently provided by licensers like: GIG Karasek GmbH, GEA Wiegand GmbH, Schulz &Partner, Tofflon Joy, Economy Process Solutions Pvt Ltd, Dedert Corporation, Technoforce.

The next step in the poly (lactic acid) production process is the pre-polymerization of the lactic acid, which occurs in section 200. Reactor R-201 has the same mechanical configuration than the evaporator E-101 and may be provided by one of the licenser previously pointed.

The low molecular weight poly (lactic acid) is depolymerized in Reactor R-301. This reactor is a horizontal evaporator which is available in the market and can be supplied by LeHeng (LH Evaporator).

The technologic viability of the process also depends on the viability of the purification method (section 400). This section allows the purification of lactide and is very important for the achievement of a high molecular weight PLA with good quality. The lactide can be purified at industrial scale with the following three methods:

- Solvent assisted purification: The crystallization with ethyl acetate and toluene is the most used method. A recrystallization with solvent followed by an azeotropic distillation also highlights as assisted purification.
- Melt crystallization: The differences of the fusion points of D-lactide, L-lactide and meso-lactide are used as method of separation. The industrial process includes 3 steps: crystallization, sweating and melting.
- Gas phase purification: The separation of the gaseous phase is produced due to the different of the boiling point of the different compounds. The lactide can be separated with inert gas or with a liquefied gas in order to remove the impurities from the melt or solid phase, respectively. The best known method is a purification by distillation where the lactide is separated from the impurities due to its boiling point.

The distillation is the chosen method for this process because, although the control of the columns is exhaustive, there are many advantages: the use of external solvents (which may contaminate the product) is avoided, the formation of solids leading to operability problems in downstream steps is also avoided, the overall efficiency of the process is improved and it is a well-known process.

There are 3 packed columns with structured packaging in section 400. Different suppliers or licensers provide this technology: Fenix Process Technologies Pvt. Ltd., Sulzer Chemtech, MTE Groups L.L.C, Finepack Structures Pvt. Ltd., GEA Wiegand GmbH, GT Technologies, Koch-Glitsch Corporate, Tinita Engineering Pvt. Ltd…

Once the lactide is purified, the polymerization of lactide takes place in section 500. There are two reactors in these section: R-501 and R-502.

Analogous technologies for reactor R-501 currently exists in the market: static mixer SMX manufactured by SULZER Co. Ltd., the static mixer manufactured by Noritake Co. Ltd., the static mixer ULTRA MIXER de KOMAX Co., Ltd.,.. There are also blade agitation systems produced by Kobelco Eco-Solutions Co., Ltd. And by Sumitomo Heavy Industries, Ltd for CSTR. [16]

Reactor R-502 has manifold technology and licensers. Some of them are shown in table 12, which includes static mixers for reactors, pipelines and more specific reactors which incorporates static mixers.

Table 12. Technology and licensers for reactor R-502. [17]

Institute/Company	Mixer/Mixer Reactor
Sulzer Chemtech	SMXS, SMXL, SMR, SMX, SMF, SMN, SMRX, SMV sulzer mixer and reactors
Chemineer-Kenics	Kenics KM and KMX reactors and HEV mixer.
Statiflo	Series 100 to 800
Fluitec	CSE-X and CSE-W
Charles Ross & Son Co	ISG, LPD/LLPD and IGH
Komax	K and M series
JLS International	Helical and High Shear
Primix	PMS, PMQ, PMX and PMV
Koflo Corporation	Series 308, 246, 250, 275, 330

The devolatilization occurs in section 600. Some technologies for devolatilization are: extruders, screw extruders, vented extruders strand devolatilizer, wiped film evaporators, falling film evaporators, rotary devolatilizers, vacuum kneaders, rotary disk devolatilizers, centrifugal devolatilizarers, flat plate devolatilizers, hot air dryers and static expansion chambers. And some licenser of this technology are: Sulzer Chemtech, Buss-SMS-canzler GmbH, Coperion …

8.2.3 Catalyzer availability

High molecular weight PLA production from lactide needs a catalyzer. Accordingly, this section introduces several types of catalyzers available for the ring opening polymerization process. This polymerization takes place inside reactor R-501 and reactor R-502, which is the reactor to be desing. All of the catalyst can be classified into three main categories: metal-containing catalyzers, organocatalyzers and bifunctional catalyzers.

8.2.3.1 Metal-containing catalyzers

- Tin-based catalysts: Tin (II) octanoate, $C_{16}H_{30}O_4Sn$, is nowadays the most commonly used catalyst for high molecular weight PLA production. The catalyst can carry out the reaction in melt state with good stability and has a low cost. However, it requires high temperatures for its operation due to insensitiveness in the presence of oxygen and other factors of the environment and is not able to control the stereochemistry of the reaction product. There are also tin salts and tin complexes which may act as catalyzer in the ring opening polymerization. [18]

- Aluminum-based catalysts: Aluminum triisopropoxide, $C_9H_{21}O_3Al$, is other widely used catalyst. It is used for the polymerization of rac-(lactide) with a coordination-insertion mechanism. It has many advantages compared with Tin (II) octanoate because produces PLA polymers with a molecular weight in a controlled and narrower range and also reduces the transesterification reactions. However, the PLA has a lower molecular weight.
- Zinc-based catalysts: This kind of catalyzers has a very low toxicity, high stability and high acidity. They are very used for ring opening polymerizations after Tin (II) octanoate and Aluminum triisopropoxide catalyzers.
- Group II metal-based catalysts: Some examples are magnesium, barium, strontium and calcium catalyzers. All of them have low toxicity and are colorless and inexpensive. Magnesium and calcium catalysts can be used for the production of PLA for medical application.
- Group IV metal-based catalysts: All of them have low toxicity and high acidity. Titanium alkoxides like the tetranuclear titanium alkoxide complex is an example of catalyzer available for this group. Other catalysts can be made of zirconium or hafnium. They are all very effective for the production of rac- lactide and L-lactide in bulk and solution polymerization.
- Iron-base catalysts: These catalysts have not good activity. For this reason, the reactions require more time and higher temperatures (which might cause racemization). Some examples are iron oxides, iron acetates and iron porphyrins.
- Copper-Based Catalysts: These catalyst, such as the iron-base catalysts, are not very active but they have goo molecular weight control. [18]

8.2.3.2 Nonmetal-based catalyzers

Nonmetal-based catalyzers can also perform reactions for the ring opening polymerization. Among them highlights the organocatalysts as the more commercially available catalyst. All of them are characterized by a strong activity, less toxicity and an exceptional control of the molecular weight and its distribution. Despite these advantages, these catalysts are strong Bronsted bases which has incompatibility with acid initiators. Moreover, the lactide purification is also required. The most used organocatalysts are nucleophilic bases, in contrast with acid organocatalysts, which are not often used. [18]

8.2.3.3 Bifunctional catalyzers

Bifunctional catalysts are defined as molecules with two distinct functional groups. One of them activates the monomer and the other activates the growing polymer chain. The bifunctional catalysts allow for the stereochemical definition and control of the final product, the polymerization process of the lactide can be controlled optimizing the reactivity and the selectivity of the reaction. Some examples of bifuntional catalysts for the PLA manufacturing are β-isocupreidine and benzyl bispidine. [18]

8.2.4 Utilities availability

In section 9.5.3 are included the services provided by the industrial polygon where the production facility has been located. The electricity, firefighting water and industrial water are provided by the polygon. However, the plant must incorporate a section for the installation of equipment for other process utilities. High pressure steam, medium pressure steam and low pressure steam must be produced inside the facilities and all of them are very typical utilities in chemical engineering processes.

8.2.5 Labor force availability

The labour force availability will depend on the location of the polylactic acid production plant. This labor force can be provided by the SEPE (“Servicio Público de Empleo Estatal”) in the Spanish territory. Moreover, websites can also be used for contacting people specialized in the field related to this process. The mobility of the population is not a problem nowadays.

Regarding to and specific location (Sagunto, as indicated in section 9 of this project), the population near the plant plot can be hired. Sagunto has an office of SEPE inside the area of the port.

9. Installation site

9.1 Site selection criteria

The site selection for the facility considered in this project is a critical decision to be made because the process profitability may depend on it. The key factors considered during the site selection are: exact location regarding marketing aspects, feedstock supplies, means of transportation, labor availability, utilities availability, land availability, environmental footprint, local community considerations, climate and political or strategic considerations. [19]

The closeness to the raw material is an important factor to take into account during the site selection. PLA is a relatively expensive product, if compared with others polymer/plastics of petrochemical base. The final PLA price will depend on the feedstock's prices, including transportation from the supplier facilities.

The chosen site must be larger enough to fulfill with the minimum plant layout requirements and also consider future expansions for the facility. However, the land size should not be excessive in order to avoid negative effects on the projects profitability.

Furthermore, the suitable land should be available for purchasing and should be affordable, with a sale price as lower as possible. To all of these, the accessibility should be added as significant aspect. The accessibility is provided by roads or rails and is required for the introduction of feedstock and the product departure.

Political stability is an aspect which is relevant in countries which support some chemical industry projects or in countries with continuous changes in certain political legislatures. [20]

9.2 Raw material supplies

The raw material to be used in the PLA production process is lactic acid. The site selection relies on the lactic acid manufacturers and suppliers. Below is shown some of the lactic acid suppliers in Spain, some of them were already mentioned in section 4.8.1 of this project.

Table 13. Some lactic acid manufactures and their location. (Own authorship).

Manufacturer/Supplier	Location
Helm Ibérica S.A.	Alcobendas (Madrid) and storage tanks in port of Barcelona.
Lluch Essence S.L.	Prat de Llobregat (Barcelona)
Purac Bioquímica S.A.	Montmeló (Barcelona)
EPSA Emilio Peña S.A.	Torrente (Valencia)
3A Antioxidants	Las Torres de Cotillas (Murcia)
Coralim Aditivos S.L.	Rribarroja del Turia (Valencia)

As shown in table 13 most of the manufacturer companies are located in Easter Spain, the Mediterranean area.

9.3 Product sale

The poly (lactic acid) has many applications, some of them are explained in section 6.1.3. There are many competitors or PLA manufacturers but most of them are not located in Spain. The main competitors were previously named in section 4.8.2., but should be highlighted NatureWorks, the mayor PLA producer in the world.

Table 14. Some Spanish poly (lactic acid) manufactures and their location.

Manufacturer	Location
Condensia Quimica S.A.	Carrer de les Jonqueres (Barcelona)
Viscofan S.A.	Tajonar (Navarra)
Purac Bioquímica S.A.	Montmeló (Barcelona)

9.4 Site selection

The poly (lactic acid) production facility is going to be located in the Parc Sagunt I which is in the town of Sagunto, in Valencia. Sagunto is situated at a distance from 24 km of Valencia, at 327 km from Barcelona, at 375 km from Madrid and 216 km from Alicante. Sagunto is at the North of Valencia and is the most important city of the Camp de Morvedre region. Nowadays, the city has 65,669 habitants (2018 data), although the demography has not changed too much. Actually, there were 56,607 habitants 20 years ago. [21]

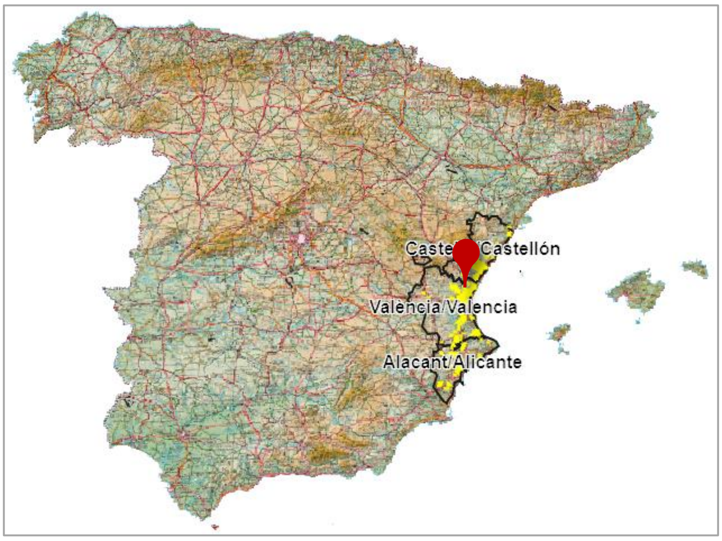


Figure 26. Parc Sagunt I location in Spain. [22]

9.5 Polygon feature

Nowadays, the Parc Sagunt I, with 3,027,859 m^2 gross, is the largest business park in Europe. The Parc Sagunt I land is classified as building land with a simple and rectangular polygon plot design in order to enable the construction of new facilities. The polygon inside roads are arranged in two lines, one on each direction, in such way to enhance the truck movement and allow easy access without traffic disruptions or any other inconvenient. The polygon can both be used for industrial or tertiary aspects: 1,022,587 m^2 are for industrial use while 165,815 m^2 are for tertiary use. The remaining ground is dotational public land and green spaces. Currently, there are 4 enterprises in the polygon and there are 15 available plots (for sale) destined of industrial character, 3 for tertiary activities and 1 for logistical activities. The plot surfaces are in a range between 8,550 m^2 and 50,001 m^2 and the square meter prices for industrial uses is 103 €.

The Parc Sagunt I have any other specific conditions: The construction of single-family homes is not allowed, unless the security guard of the facilities stays there, the polygon building is characterized by single isolated plots and the maximum suitability for buildings is 0.638 m^2 per square meter build. [21]

Some constraints are imposed during the facility building process in this polygon industrial area and these are determined according to planning requirements. In table 15 are shown some of these constraints.

Table 15. Parc Sagunt I constraints for building construction. [21]

Attribute	Description
Typology	Single building
Buildability	1.05 m^{2}t/m^{2}s
Cornice height	15 m, except in duly justified cases in which the height is 35 as maximum.
Maximum overall height	3.5 m higher to the building cornice height. In justified cases the height may reach a value of 10 m.
Maximum number of plants	4, although in justified cases the maximum number of plants is 7.
Maximum occupancy	70 % over the net plot.
Retreats	The buildings must keep 10 m distance to the road and 6 m to the rest of the boundaries.
Construction flights	Forbidden over retreats and roads.
Minimum surface of plots of land	Minimum surface of 6000 m^2 with a minimum length of 50 m, in general.
Permitted uses	Industrial, garages y workshops, department stores, complementary offices, shows and recreation centers and equipment.

9.5.1 Land plot location

The Parc Sagunt I polygon is located in an area where new and already well-known polygons coexist. Parc Sagunt II can be stand out as a modern polygon while "Polígono Químico" and "Polígono Industrial Siderúrgico" are historical polygons settle a few years ago. In Figure 27 are shown neighboring polygons.

Figure 27. Parc. Sagunt I neighboring polygons. [22]

As previously mentioned, the chosen polygon has many plot lands for sale. The selected one has the characteristic shown in table 16.

Table 16. Plot land details. [21]

Reference	I-6.5
Availability	Available
Purpose	Industrial
Area	15,553 m^2
Plot occupancy coefficient	70%
Building coefficient	1.05 m^2
Sale price	1,601,959.00 €
Cadastral reference	4915405YJ3941N
Coordinates	Latitude: 39º 38' 19.5'' N Longitude: 0º 15' 52.0'' W

In figure 28 is illustrated the Parc Sagunt I polygon via satellite. Moreover, in the figure is more or less indicated how close is found to the Sagunto´s port.

Figure 28. Parc. Sagunt I via satellite. [23]

In Figure 29; instead, the available plot lands are shown. In light blue color the plot lands for sale are highlighted and in yellow is indicated the chosen plot for this project.

Figure 29. Parc. Sagunt I plot lands representation. [21]

9.5.2 Communication routes

9.5.2.1 Road network

The most important communication roads are: AP-7, A-7 and A-23. The first one link Sagunto with Valencia, the second one, Sagunto with Castellón de la Plana and the third one Teruel with Zaragoza. On the other hand, some secondary roads can be named. N-234 and N-340 runs in parallel with A-23 and A-7 and are other options to arrive to Teruel and Castellón de la Plana.

The CV-320 is a community road which communicates the Parc Sagunt polygon with the Sagunto city. The CV-309 is link to the CV-320, which is from Valencia. There are others like CV-317 (Sagunto town- Canet d´En Berenguer-Almardá), CV-3202, CV-3201, etc. [24]

9.5.2.2 Maritime communication routes

The Saguntos´port is located at 22 km from Valencia and is integrated into the Valencia Port Authority. This port authority is classified as one of the 10 first port authorities in Spain according to the freight traffic. In 2017 the Valencia Port Authority was the second one, because of the high volume of freight transport (around 3.24 million tons). The Sangunto´s port has a total Surface of 1,459,897 m^2 and has a refrigerated warehouse of 65,000 m^3. Moreover, there are two commercial basins with a 200 Ha water mirror.

The Saguntos´s port is directly connected to the Spanish motorway by means of V-23 and CV309. The highway A-23 is needed then to continue northwards. The A-7 motorway, which in turn links to the A-25 motorways is required for north-South Corridor movement. Besides, the V-21 allows for the Valencia coast circulation. [25]

9.5.2.3 Rail Network

As shown in figure 30, there´s a freight terminal for the Sagunto´s port.

Figure 30. Freight transport by railway in Valencia and surroundings. [26]

9.5.2.4 Air communications

The closest airport is located in Valencia and is at 36 km from the Sagunto´s port. The estimated trip by car is about 29 minutes and AP-7 and V-23 are the roads needed to make the journey. The Valencia airport has a great significant because contributes to the staff mobility, although for merchandise transportations are better the other means of communication.

9.5.3 Services

The Parc Sagunt I have the services shown below:

- Electricity: High, medium and low voltage with a park´s own substation. The supply is 40 W/m^2 (20 kV).
- Potable water: The supply is 0.2 l/s·ha
- Industrial water: Ths supply is 0.8 l/s·ha
- Fire protection water supply: In storage
- Natural gas: ERM 2500 m^3/h APA 25 bars BP
- Communications: telecommunication, phone network, optical fiber cable.
- Skilled labor: Coming from the Sagunto city or from Valencia, located 24 km away.
- Other services: Local police surveillance, public parking area with 6,458 parking bays and private parking areas with 12.916 parking bays. There´s also a sewage treatment plant and a waste collection system (SAG, "Sociedad Anónima de Gestión). [21]

9.5.4 Future expansion

In 2018, Parc Sagunt I had reached an 80% occupation level. The industrial and commercial activity in the area seems to set growth and the plot lands which were not sold are much demanded. Currently, and as shown in figure 29, there are several plot lands in the surroundings of the chosen plot land. For this reason, a mayor scale enlargement can be possible. Because of the high demand, how much time will be the lands available is unknown. The chosen plot land has already taken into account possible enlargements in a more distant time. However, if the considered expansion is for a new section for the facility (for example, a new storage area for products or raw materials) then, a new land purchasing may be considered. The purchased land might be located in the newest Sagunto City Council industrial project, Parc Sagunt II. Furthermore, the empty plot lands in the surrounding polygons may be considered.

9.5.5 Political and strategic considerations

The proximity to suitable raw material is the factor which was initially considered for the PLA production facility site selection. In table 13 are shown some lactic acid suppliers, although there are many others. The supplier's location analysis provided information indicating that most of them are located in Cataluña, and a few others are mainly sited Valencia and Madrid.

Regarding to political considerations, Cataluña is not a good option for the facility site selection. On 6 October 2017 the Spanish government approved a decree facilitating the relocation of the business headquarters. This action was the result of the outlawed referendum of independence in Cataluña. The political situation has been, ever since, unstable and has led to the relocation of many companies. Many enterprises moved to Madrid, Valencia and Andalucía. For all this reason the PLA facility could not be sited in Cataluña.

Valencia, and especially the Sagunto City Council, sets out a stable policy which helps to economic growth. The economic reactivation may be achieved with the construction of new polygons to attract new companies and with good communication infrastructures. Additionally, Parc Sagunt I, is located in the center of world maritime trade, which makes the location ideal for business and logistics activities.

In addition to the previous explained strategic and political remarks, the national market was considered. The biodegradable packaging manufacturing for the foodstuff sector is one of the PLA applications. Food and beverage industry are the first billing industry sector in Spain, being the fourth country in the European Union. According to business number Cataluña, Andalucía, Castilla y León and Autonomous Community of Valencia are the key Spanish communities in the food sector. In such way, Sagunto is located in the national exportation center.

9.5.6 Climatology

9.5.6.1 Precipitation

The Autonomous Community of Valencia had a normal precipitation range between 0 to 100 mm per month in the last 30 years. The precipitation diagram for Valencia is shown in figure 31. According to this figure, the weather is quite dry and typically do not rain more than 3 days per month. Besides, the precipitation is not often larger than 2 mm.

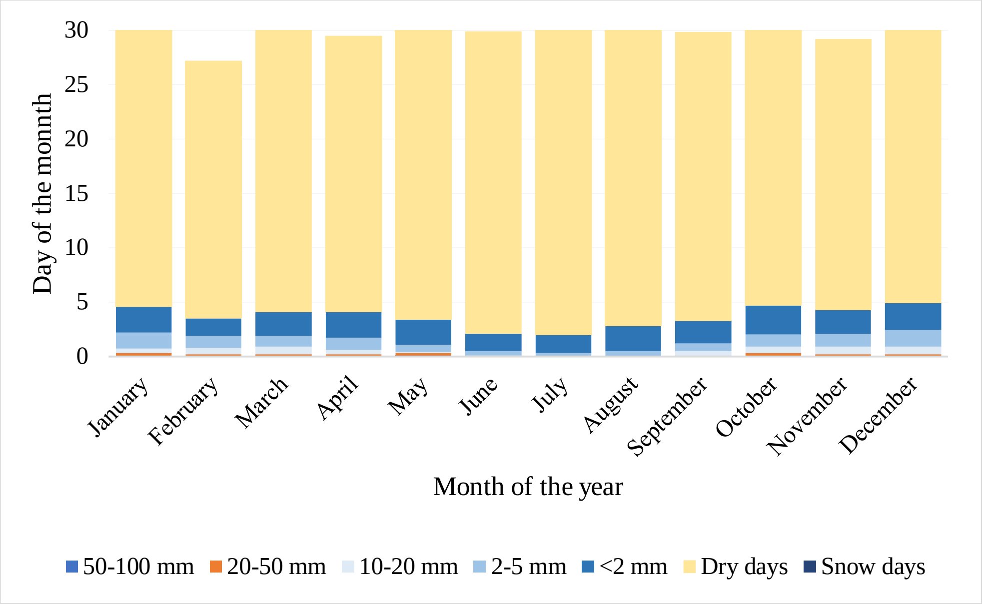


Figure 31. Monthly precipitation average of the last 30 years. [27]

Data collected between 1989 and 2010 indicates the following:

- The average annual rainfall was 475 mm.
- The average relative humidity was 65% for a year.
- The average of days with precipitation equal or higher than 1 mm was 46.3.
- The average number of days for a year when there is snowing, storming, fog, and freezing are 0.1, 15.3, 5 and 0.5, respectively.
- The average sunny days was 93.2 [28]

Despite of the previous average data, many other meteorological phenomena might happen. Some of them were collected since 1937 and can be observed in table 17.

Table 17. Meteorological maximums and minimums for precipitations. [29]

Attribute	Value	Date
Maximum rainy days per month	21	October 1990
Maximum days of snows per month	3	December 1946
Maximum days of storms per month	10	October 1986
Maximum rainfall during one day (l/m^2)	262.2	17 November 1956
Maximum rainfall during one month (l/m^2)	365.6	October 1965
Minimum rainfall during one month (l/m^2)	0.0	September 2013

9.5.6.2 Temperature

The Community of Valencia has very hot summers with sunny days and long, cold, cloudy and windy winters. Keeping this in mind, the higher temperatures are between 6ºC and 30ºC and the lower ones are in a range between 2ºC and 33ºC. The listed average temperature since 1981 to 2010 was 18.3ºC. Between these years, the maximum dairy temperature was 22.8ºC and the minimum was 13.8ºC. The maximum temperature diagram in Valencia is shown in figure 32.

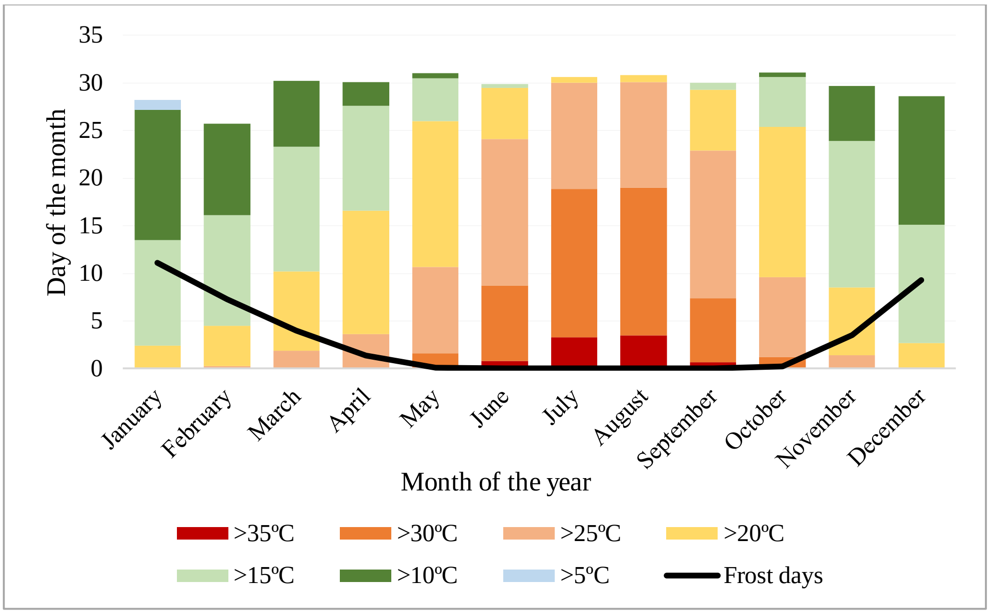


Figure 32. Monthly maximum average temperatures of the last 30 years. [27]

Just like with precipitation, many other meteorological phenomena related to temperatures aspects might happen. Some of them are collected in table 18.

Table 18. Meteorological maximums and minimums for temperatures. [29]

Attribute	Value	Date
Maximum absolute temperature (ºC)	43	27 August 2010
Minimum absolute temperature (ºC)	-7.2	11 February 1956
Highest average temperature (ºC)	28.1	August 2003
Lowest average temperature (ºC)	6.2	February 1956
Maximum of the average temperatures (ºC)	33.1	August 2003
Minimum of the average temperatures (ºC)	0.9	February 1956

9.5.6.3 Wind

The maximum wind velocity was recorded the 25 February of 1989 according data collected from 1945 to 2012. The wind reached a value of 117 km/h. However, this is not a normal value in Valencia Community. The normal wind velocity is around 15 km/h. The wind velocity of the last 30 years is shown per month in the wind velocity diagram indicated in figure 34.

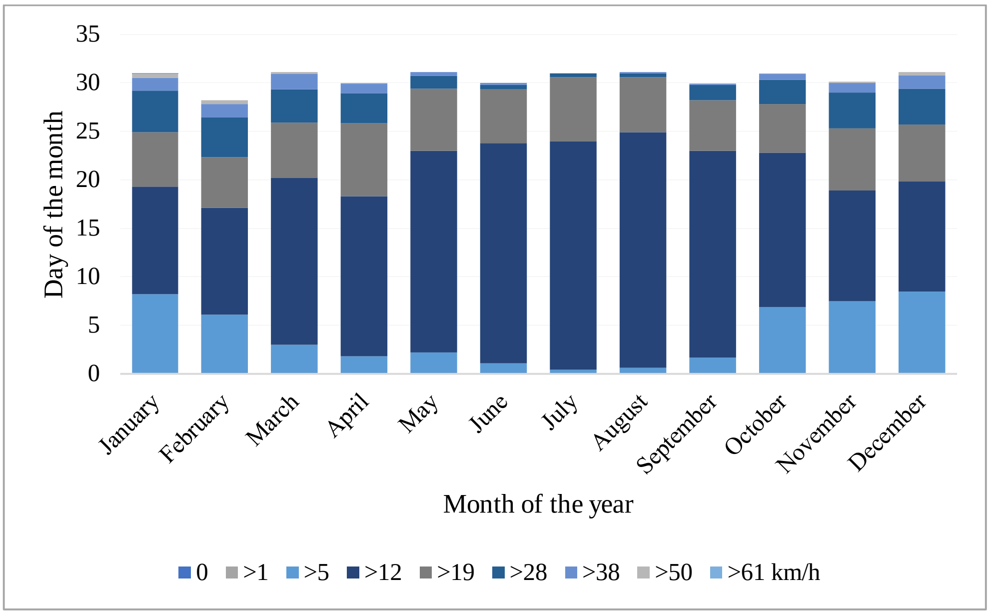


Figure 33. Monthly maximum average wind velocity of the last 30 years. [27]

9.5.7 Seismicity

The PLA production facility site selection also has taken into account the seismic activity. A high magnitude earthquake can compromise the facility structural integrity giving to hazard situations, with equipment and pipeline breakage, in which there is an uncontrolled chemical released.

The Iberian Peninsula is located close to the contact zone of two colliding lithospheric plates, Eurasian and African plates. The seismic activity is produced by the movement between them. The activity is higher in this area (southern Andalucía). Even so, there is also a high seismic activity in the Pyrenees. [30]

The Autonomous Community of Valencia is placed between the previously named areas. The seismic intensity is not too elevated, especially in the north of the community. Data for the coming 100 years in the Iberian Peninsula is shown in figure 35.

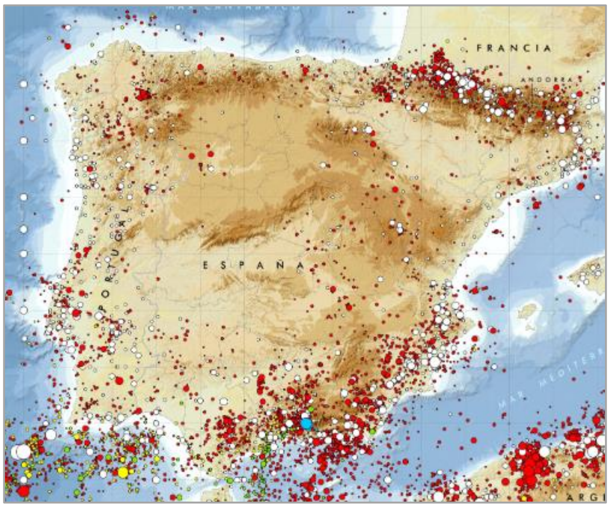


Figure 34. Seismic Hazard map, 2015. [31]

9.6 Justification for the installation site selection

The PLA production facility is located in the Autonomous Community of Valencia, in “El camp de Morvedre” district and in the Sagunto´s municipality. The location site selection has taken in mind the closeness to the raw materials, which are mainly placed in Cataluña, Madrid and the Community of Valencia. All of these places where considered initially. Cataluña, has a very strong chemical industrial sector since many years ago, but nowadays the region is suffering from economic instability which was caused by a political instability. The facility was not placed in Cataluña because the lasting time of the instability is unknown. Madrid was not selected too. The main reason were the high industrial land price and the increasing costs for trade with foreign countries. The chosen location has advantages of strategic-commercial character and is an area with economic growth. Moreover, the Parc Sagunto I, is new-built and has updated technologies in compliance with current standards.

10. Process description

In this project´s section is described by sequential order and plant section the operations involve in the lactic acid transformation to produce poly (lactic acid). The production process is carried out continuously with a 330 days operating time period. The lactic acid is the only raw material needed for this process and is considered to be a combination of D-lactic acid and L-lactic acid, its optically active enantiomers.

The indicated process sequence is required for the production of a high molecular weight polylactic acid of high purity. Low molecular weight polylactic acid can be obtained in a process where only two sections or steps where required (raw material treatment and polycondensation reaction). However, the process considered in this project is a little bit more complex.

10.1 Installation description

The production of high molecular weight polylactic acid has a total of 6 sections.

- Section 100: Lactic acid pretreatment or raw material conditioning.
- Section 200: Pre-polymerization of polycondensation reaction.
- Section 300: Lactide formation.
- Section 400: Lactide purification.
- Section 500: Polymerization reaction or ring opening polymerization.
- Section 600: Volatilization.

The process and the equipment will be described for each plant section in the next sections of this project. The block diagram of the process gives an idea of the magnitude of this project and is provided in figure 35.

Apart from the battery of the process, this facility also has a laboratory building, a control room, an area for the storage of raw materials and products, and area for the utilities, and area for the treatment of the waste, a parking area, an office building and a security building. All of this information is provided in Document II. Plans.

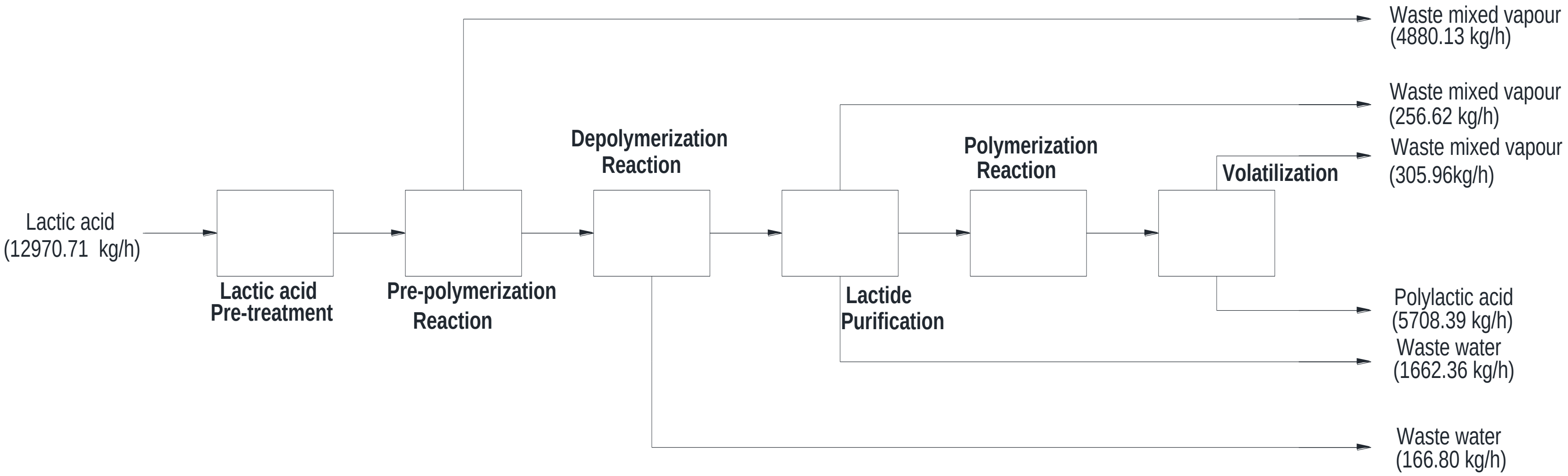


Figure 35. Process block diagram of the polylactic acid production process. (Own Authorship)

10.2 Process description

10.2.1 Section 100: Lactic acid pretreatment

The main raw materials, in this case only lactic acid, are storage initially in a tank at atmospheric pressures and temperatures between 15-25ºC, more specifically 20ºC [32]. Lactic acid is liquid at this particular conditions because its boiling point is at 215ºC. The aqueous solution of 80%wt lactic acid is pumped to a pre-treatment section. The inputs characteristics of lactic acid where explained above in section 5.1.3. The lactic acid is, then, introduced in the evaporator E-101 for further concentration of the aqueous solution feed and for some volatile impurities elimination. During the evaporation, water and some other impurities like methanol are being removed [33].

The mayor content of water must be removed in order to avoid hydrolysis reactions when the reactive process in the pre-polymerization reactor, depolymerisation reactor and polymerization reactors takes place. These set of reactions will reduced considerably the molecular weight of the polymer.

For this reason, lactic acid is concentrated until 98.5%wt. The evaporator operates at 95ºC and 6.5 kPa, so for this particular case the racemization phenomena can be considered negligible. For higher temperatures and pressures the racemization may be between 1-10% with respect to the more concentrated enantiomer [34]

When the evaporation comes to an end, the concentrated lactic acid is pumped to the pre-polymerization reactor R-201.

10.2.2 Section 200: Pre-polymerization reaction

Before the concentrated lactic acid can be introduced in the pre-polymerization reactor R-201 the temperatures and pressures must be adjusted. The pressure is increased until 350 mbar and the temperature, until 140ºC, so the feed of the reactor is liquid. In the R-201 reactor, lactic acid is transformed by self-esterification into a 2500 g/mol poly (lactic acid) and water. In other words, a polycondensation takes place. Side reactions may occur and by-products like lactide and lactic acid esters can be formed. However, side reactions in this reactor are going to be considered negligible because, although they cannot be inhibited, most of the impurities are removed before lactic acid enters this reactor. [33]

Lactic acid polycondensation is a reversible reaction and, for this reason, the progress of the reaction occurs when the by-product (water) is eliminated. The water removal increases the reaction rate and the conversion.

During the polycondensation, lactic acid monomers are linked with an ester bond which can break under inappropriate process conditions in order to form cyclic molecules like lactide. This is the description of depolymerisation, which for this reactor is a side reaction. Accordingly to all of this, the chosen pressures and temperatures contributes to the reduction of depolymerisation. [35]

Reactor R-201 operates at 180ºC under inert atmosphere because conversion increases with temperature. However, there are two limits. Temperatures below 120-135ºC are not possible because the lactic acid self-esterification starts in this range of temperatures. Temperatures beyond 230-260ºC are also impossible, at this temperatures poly (lactic acid) starts its thermal breakdown. [12]

The reactor stream outlet is a liquid-melt phase of lactic acid polymer, lactic acid, water and non-volatile impurities. At the reactor operating pressure lactic acid boiling point is 186.31ºC and poly (lactic acid) melting point is between 150-160ºC. Water is mainly removed with the vapor, however a part is retained in the liquid-melt phase. This stream is pumped to a stirrer storage tank at 160ºC. Besides its high boiling point, lactic acid remains in liquid phase also because it's low volatility, its low vapor pressure and the mass transfer resistance due to the polymer formation. [36]

10.3 Section 300: Depolymerization reaction

The liquid-melt phase of low molecular weight poly (lactic acid) is mixed with a catalyst (stannous octoate) and a stabilizer (thimethyl phosphite) in the stirrer storage tank. The stabilizer contributes to the reduction of the racemization of the lactic acid remaining in the product and the lactide ring.

The amount of catalyst and stabilizer added to this tank must be sufficient enough in order to assure the concentration of both, in the inlet stream to the reactor (stream 22), as 0.1%wt and 0.03%wt respectively. [33]

The mixture from the stirrer storage tank V-301 is pumped to the depolymerisation reactor, which is operating at 2.5 kPa and 220ºC.

The lactide is formed by a melt polymerization process where the polymer is transformed via backbiting reaction. The reaction is reversible and depend on an equilibrium where the heat transfer, mass transfer, pressure and catalyst concentration plays and important role. [37] The crude lactide product obtained is vaporized while the reaction is performed and the equilibrium is continuously shift to the formation of more lactide.

The mass transfer is favoured at low pressures and the heat transfer depends on the operating temperatures and the heat required by the reaction. Although this reactive system can operate in a range of temperatures of 180-300ºC, 220ºC is a temperature which considers the reaction rate, the degradability of the poly (lactic acid) and the reaction requirements (endothermic reaction).

The depolymerization reactor has two outlet streams. There is a vapour stream with a composition of 91.5%wt of lactide (L-lactide, D-lactide and meso-lactide), a 5%wt of oligomers, a 2.5%wt of water and a 1%wt of lactic acid. The liquid stream consists of a mixture of poly (lactic acid), non-volatile impurities, catalyst and stabilizer. Most of the poly (lactic acid) has not reacted and converted to lactide. In order to recover this material, a recycle has been made and the liquid stream outlet of the depolymerization has been introduced in the stirrer storage tank V-301. Moreover, a purge is required for the elimination of non-volatile impurities, catalyst and stabilizer. Without a purge, the impurities will accumulate in the reactor during the steady state operation and the probability of side reactions sharply increases.

10.4 Section 400: Lactide purification

The vapour stream outlet (stream 23) of the reactor R-301 must be fed to a purification system before the lactide can be polymerized and formed high molecular weight poly (lactic acid). The purification system consists of 3 distillation columns (Columns T-401, T-402 and T-403). Columns T-401 and T-402 are required for the purification of lactide and elimination of impurities like water, lactic acid and oligomers (two unit poly (lactic acid) or dilactic acid). Column T-403 is used for the separation of the lactide enantiomers (L-lactide, D-lactide and meso-lactide). L-lactide and D-lactide have very similar properties and the separation with a distillation column is not possible. Both enantiomers are separated from meso-lactide.

The crude lactide coming from the depolymerisation reactor and with the appropiate conditions is fed to the column T-401. This column operates at 2 kPa and the separation is made to obtain lactide in the bottoms and other more volatile components like water, lactic acid and dilactic acid in the top. Lactide is the less volatile component to be separated.

The bottoms product has a composition of 98.74%wt of lactide, the vapour distillate has a composition of 32.48%wt of lactide and the liquid distillate has a composition of 91.84%wt of lactide.

The liquid distillate of the column T-401 is the feed of the column T-402. The operation of column T-402 is similar to the previously explained column. The bottoms product has a 99.7wt% of lactide, the liquid distillate 53.97 %wt and the vapour distillate 10.12 %wt.

The bottoms product obtained in columns T-401 and T-402 is mixed and fed to the column T-403. In this column de meso-lactide is separated from the L-lactide and the D-lactide. The meso-lactide is obtained in at top of the column with the remaining impurities of lactic acid. The meso-lactide content in the bottoms product is 0.01, which is smaller than the value of 0.05 recommended in bibliography. [38]

10.5 Section 500: Polymerization reaction

The purified lactide must be then introduced in the reactor R-501 where the ring opening polymerization of lactide starts. Inside this reactor are mixed the catalyst (stannous octoate) and the co-catalyst (1-dodecanol) with the lactide stream 51 in such way that the input concentration to the reactor of both components is 0.014%wt and 0.34%wt respectively. The feed to reactor R-501 mainly consists of L-lactide. Then, and in accordance with the enantioselectivity, the high molecular weight poly (lactic acid) formed is isotactic and its structure is crystalline. The tacticity is characterized by a monomer bond formation of type –L-L-L-. [39]

In agreement with some comercial patents, the lactide polymerization reaction must be carried out in a temperature range of 100-240ºC and in particular between 180-210 ºC because the reaction takes place without solvent and in melt phase [40]. Beyond 250 ºC the polymerization can be uncontrolled and the depolymerisation reactions becomes more significant. For all this reasons the operating temperature is 180ºC.

The pressure is not a critical variable. During polymerization the pressure should be enough to make flow the reactant liquid/melt mixture.

The polymerization of lactide to poly (lactic acid) is not only performed in the reactor R-501. In fact, this polymerization must be carried out in two steps: one step for low molecular weight polymerization and other step for high molecular weight polymerization.

The first step is happening in reactor R-501. The reactant mixture reaches a low viscosity at the final conversion is 0.459 for a final molecular weight of the polymer of approximately 66100 g/mol. The polymer/lactide mixture is introduced in reactor R-502, where the second step takes place, for higher conversions. The final conversion is 0.95 with a final polymer of 136970 g/mol of molecular weight. Higher conversions cannot be achieved due to thermodynamic and product specification reasons at the operating temperature.

The residence time for polymerization is 3.5 h, time at which a reasonable conversion is achieved. This residence time is between a range of 15 min and 6 h. Residence times lower than the indicated in this range are not enough for the attainment of the desire poly (lactic acid) and higher residence times contributes to the discoloration and the increase of the dispersion degree of the polymer. [41]

Once the polymerization reaction has finished and, in order to prevent possible depolymerisation reactions like degradation or hydrolysis, a deactivating agent is added to the poly (lactic acid). The phosphoric acid is the deactivating reagent added and is 0.05-0.08 times the amount of catalyst. [42]

A stabilizer agent must also be added to the product to prevent the loss of molecular weight of the polymer during the step of devolatilization. The amount of this agent is 0.0083 %wt and is 2,6-di-t-butil-4-metilfenol due to its low volatility. The deactivating and stabilizing agents are going to be mixed to the poly (lactic acid) with an extruder. Finally the lactic acid is pumped to the devolatilization step.

10.6 Section 600: Devolatilization

Once the polymer is formed, stabilized and deactivated, must be summitted to a devolatilization step in order to remove volatile components like the lactide. These components are eliminated with high temperatures and low pressures. For this reason this step is performed at 220 ºC and 6.5 kPa. The final polylactic acid has a concentration of 0.009 wt% of impurities. The separation of the more volatile impurities take place in the flash vacuum chamber V-601. [43]

11. Equipment description

This section of the project gives some details of the description of the equipment required for the process to be carried out. The description can be categorized depending on the function of the equipment into main equipment and auxiliary equipment.

11.1 Principal equipment of the process

11.1.1 Lactic acid storage tank TK-101

This equipment contains lactic acid at 20ºC and atmospheric pressure. This storage tank is provided by a heating system in order to avoid temperatures lower than 15.5ºC, which is the lactic acid freezing point, during cold winters. It has also a refrigeration system because a temperature increase may lead to the formation of lactic acid vapours resulting in explosive mixtures that may react with air. The tank is located surrounded by a retaining wall for prevention or safety measure in case of possible leaks.

11.1.2 Evaporator E-101

The lactic acid pre-treatment is performed in an evaporation system integrated by a single falling film evaporator. This evaporator works at 6.5 kPa and reaches a temperature of 95ºC. As indicated, the evaporator operates with vacuum pressures and very low residence times, so the heat sensitivity of the materials are considered. The liquid aqueous solution of lactic acid enters the evaporator at 20ºC and when is flowing down as a thin film through the heat exchanger, the solution becomes a two-phase stream, which enter a separator for the liquid and vapour state phases disaggregation.

The main components of this evaporator are the heat exchanger, the separator, the empty systems, piping and control instrumentation. In this evaporator lactic acid is introduced at 80% wt and due to its low pressure and temperature the racemization of the L-Lactic acid to D-Lactic acid is not taking into account. The racemization phenomena sharply increases with temperatures above 180ºC.

The tables 2 and 3 shown in this descriptive report compile some information related to the boiling point of lactic acid at 6.5 kPa and for a 0.8 of mass fraction. Lactic acid boils at 140ºC for this composition and boils at 150ºC for a 98.5% lactic acid. At 95ºC and the expected final concentration, a 5% of the lactic acid is lost with the vapour and is pumped to wastes treatment. This vapour has a composition of 18%wt of lactic acid, which is very high and the possibility of further treatment of this stream for lactic acid recovery could be considered.

In addition to the previously explained, some information about the composition of the construction materials of the evaporator must be indicated. The lactic acid is a corrosive material, especially at high temperatures. For this reason, the evaporator is made of austenitic stainless steel, although other materials such as nickel alloys or ferritic alloys can be used. [44]

11.1.3 Pre-polymerization reactor R-201

The step-growth polycondensation of lactic acid is produced in a reactor with a falling film evaporator configuration. This type of reactor allows the formation of a thin film of liquid over the tube walls, which clearly enhance the mass transfer rate. Moreover, the water by-product formed during the reaction can be continuously removed.

It is a very versatile equipment with very short residence times and a good control of the operating conditions. This reactor also reduces the racemization. Nevertheless, a 5% of the L-Lactic acid enantiomer is converted to the respective D-Lactic acid enantiomer because of the pressure and temperature conditions. This reactor operates at 35 kPa and reaches a temperature of 180ºC. Inside the reactor there is a temperature slope because the sudden increase in temperature can degrade the reaction medium, so, the inlet temperature is 140ºC [45]. It operates at non-isothermic conditions because it cannot be considered as adiabatic or isothermic. At adiabatic conditions the reactor would reach a temperature of approximately 282ºC.

11.1.4 Stirrer storage tank V-301

This vessel has the physical conformation of CSTR and has a cooling jacket in order to remove the heat from the hottest streams introduced in the system. This vessel has being installed in the process in order to mix the catalyst and stabilizer but also to improve the controllability of reactor R-301. The residence time is increase and the recycle stream can be better controlled without increasing losses of polylactic acid through the purge stream 26.

11.1.5 Depolymerization reactor R-301

The lactic acid, poly (lactic acid) and lactide are very heat sensitive materials. For this reason, the configuration of the depolimerization reactor R-301 is going to be similar to an evaporator. This configuration is also required for the removal of the vapour lactide product. In particular, R-301 reactor is a horizontal tube evaporator. The lactide vaporizes over the horizontal tubes due to the heat transfer of hot condensing vapour flowing inside the tubes. Although other type of configuration reactors like falling film evaporator configuration can be chosen, this reactor has many advantages: low retention times, high heat transfer coefficient, great area for separation by unit volume, low hydrostatic loss in the head, low headroom and descaling capacity. [46]

11.1.6 Column T-401

Column T-401 operates at 2 kPa and a temperature of 144 ºC in the top and 152 ºC in the bottoms and the feed is at 100 ºC. Column T-401 is a distillation column with a structured packed bed. The configuration of the column is required due to the very low pressure and the high temperatures. Furthermore, the liquid hold up is minimized, so the racemization and the pressure drop in the column is reduced. The packed column configuration also contributes to the minimization of possible side reactions to occur.

The column operates with a partial reboiler and a mixed condenser. The distillate is then, liquid and vapour and the bottoms product is liquid. This column cannot operate with a total condenser because at the operating pressure the water boiling point is 17.5 ºC. The vapour leaving the column at the top is a mixture, so the vapour will be totally condensed when all of the components of the mixture are condensed. The reflux ratio for this column is 0.6 and the distillate is at 112 ºC.

11.1.7 Column T-402

Column T-402 is similar to column T-401. It is a packed bed column operating at 2 kPa. The feed of the column is 112 ºC, the distillate is at 112 ºC and the bottoms are at 153.6 ºC. The reflux ratio of this column is 6 and also operates with a partial reboiler and a mixed condenser.

11.1.8 Column T-403

Column T-403 is a distillation packed column operating at 2 kPa. The feed of the column is at 120 ºC. The temperature of the distillate is 132.81 ºC and the temperature of the bottoms product is 141.82 ºC. This column operates with a total condenser and a partial reboiler. It is also, just like columns T-401 and T-402, a multicomponent distillation column. The reflux ratio is 0.6.

11.1.9 Reactor R-501

Reactor R-501 is small stirrer storage refrigerated with cooling water with a cooling jacket. Its volume is 2.82 m^3 and its main objective is the mixing of the catalyst with the lactide while obtaining a conversion of 0.459 to polylactic acid.

11.1.10 Reactor R-502

This reactor is a PFR because can handle with high viscosity at the same time the heat is efficiently removed. More information of this reactor is provided in Annex II. Supporting calculations because is the reactor which is going to be design for this academic project.

11.2 Auxiliary equipment

The auxiliary equipment is the support of the principal equipment allowing the transportation of the fluids from one equipment to another, heating or cooling the different streams to adjust the conditions of the process, creating vacuum, increasing the residence time or separating two phases. The pumps, ejector, vapour-liquid phase separators and all type of heat exchanger are included on these category.

11.2.1 Pumps

There are two types of pumps in these process. The typical centrifugal pumps and the gear pumps. All of the pumps contributes to the movement of the fluid to one equipment to another, although there are some which are also increasing the pressure.

The centrifugal pumps are: P-101 A/B, P-102 A/B, P-401 A/B, P-402 A/B, P-403 A/B, P-404 A/B and P-405 A/B.

The gear pumps are: P-201A/B, P-301 A/B, P-302 A/B, P-501 A/B and P-502 A/B.

Pumps P-102 A/B and P-302 A/B increases the operating pressure. In the first case the pressure is increased from 6.5 kPa to 35 kPa and in the second case the pressure is increased from 2.5 kPa to 350 kPa.

11.2.2 Heat exchangers

There are different types of heat exchangers in these process. All of them can be classified according to their function and to their physical configuration. All of the heat exchanger will be described through this project when calculating their energy balances in Annex I and when introducing a simple estimation of their dimensions of in Annex II.

11.2.3 Vapour-phase separators

V-401, V-403 and V-405 are auxiliary equipment required for the operation of the columns T-401, T-402 and T-403.

V-101, V-402, V-404 and V-601 are vapour phase separation required in the vacuum system. All of them are removing the liquid stream and the vapour can be reintroduced in the second ejector of the vacuum system. Their main function is the reduction of the load in the second ejector, so as cost due to the high pressure steam required for operation.

11.2.4 Ejectors

There are a total of 10 ejectors. All of them are steam jet ejectors operating with high pressure steam as motive fluid. More information of the ejectors is provided in Annex II: Supporting Calculations.

12. Safety in design and operation

12.1 Introduction

Any chemical industrial facility, like the one to be treated in this project, should be design in such a way that possible risks associated with its operating conditions are avoided. The goal is to prevent industrial accidents. For this reason, some considerations should be taken into account during the design and the facility operating time: operating conditions (temperature, pressure …) and type and amount of material to be found in the facility.

Accordingly, security shall be improved with a dangerous materials reduction, enforcing the distances inside de facility (also over the closest populations), keeping ready the protection systems (such as relief valves, for example) and taken appropriate prevention and minimization measurements.

As explained above, in this section of the project is intended to perform a series of analysis from which different aspects in the field of security have to be known. In a first step, an inventory of the chemical substances intervening in the process must be undertaken in such way that all of the involve substances can be properly classified, so as a classification of the facility. Within this context, the CLP regulation and the Seveso III Directive have especial significance. The substances collected in the inventory could also be needed for an uncontrolled chemical reactivity study. From this study is known how the different substances react respectively with each other and other components. The study can be performed according information given by the NFPA association or with an analysis of the possible reaction with reactant groups. A risk analysis for the facility has also to be added to all of this analysis. This kind of analysis can be performed according to the "what-if" methodology. As result from this analysis, some decisions related to the preventive and minimizing execution measures can be taken. Finally, the distances between the different equipment shown in this project can be calculated. Taking a minimum distance between equipment the industrial design of the facility can be consider to be intrinsically safe.

12.2 Facility classification

12.2.1 Chemical inventory

In the polylactic acid production process the following reactants, products, wastes materials and intermediate products can be distinguished:

- Lactic acid (Mainly L-lactic acid and D- Lactic acid)
- Lactide (L-Lactide, D-Lactide and meso-Lactide)
- Water
- Polilactic acid (mainly isotactic polylactic acid)
- Dilactic acid
- Methanol

All chemicals are intrinsically hazardous. Therefore, the hazards for the chemicals named above are needed to be known. The hazard for a substance or a mixture can be defined as a potential characteristic to cause harm and depends on the intrinsic property of the substance or mixture. According to this, the aforementioned chemicals properties related to the security field are collected on tables 19, 20 and 21.

Table 19. Some important properties for the process safety. (Own authorship).

Property	**Lactic acid**	**Lactide**
Boiling point at 101.25 kPa (ºC)	215	266
Specific gravity	1.22	1.09
Vapor pressure at 25ºC (kPa)	$4.73 \cdot 10^{-4}$	$3.8 \cdot 10^{-3}$
Flash point (ºC)	112	150
Self-ignition temperature (ºC)	Not pertinent	Not pertinent
Lower explosion limit (LEL) (% volume in air)	Not pertinent	Not pertinent
Upper explosion limit (UEL) (% volume in air)	Not pertinent	Not pertinent

Table 20. Some important properties for the process safety (continuation). (Own authorship).

Property	**Water**	**Poly (lactic acid)**
Boiling point at 101.25 kPa (ºC)	100	Not pertinent
Specific gravity	1	1.24
Vapor pressure at 25ºC (kPa)	3.17	Not pertinent
Flash point (ºC)	Not pertinent	Not pertinent
Self-ignition temperature (ºC)	Not pertinent	388
Lower explosion limit (LEL) (% volume in air)	Not pertinent	Not pertinent
Upper explosion limit (UEL) (% volume in air)	Not pertinent	Not pertinent

Table 21. Some important properties for the process safety (continuation).

Property	Methanol	Dilactic acid
Boiling point at 101.25 kPa (ºC)	64.53	215.88
Specific gravity	0.78	1.38
Vapor pressure at 25ºC (kPa)	16.82	$1.25 \cdot 10^{-4}$
Flash point (ºC)	12	Not pertinent
Self-ignition temperature (ºC)	385	Not pertinent
Lower explosion limit (LEL) (% volume in air)	6	Not pertinent
Upper explosion limit (UEL) (% volume in air)	36	Not pertinent

12.2.2 Classification according to CLP regulation

Regulation (EC) No. 1272/2008 on classification, labelling and packaging of substances and mixtures, also named as CLP, incorporates into Community legislation the requirements contained in the Global Harmonization System (GHS). CLP allows for the identification of hazardous chemicals and the communication of these hazards to users through labelling. It also allows for the hazard substance or mixture classification if one or more class or hazards are being contemplated according criteria shown in the CLP. For the substances previously named on the chemical inventory collected for this project in section 12.2.1 must be determined their hazard classification. There are hazard classes for physical hazards, health hazards and environmental hazards.

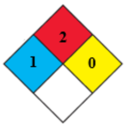
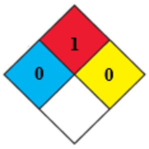
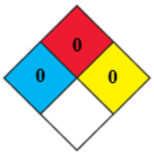
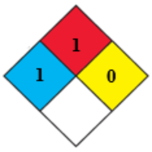
The CLP Regulation replaces previous rules on classification, labelling and packaging substances (according to Directive 67/548/EEC) and mixtures (according to Directive 1999/45/EC). It also provides the basis for safety data sheets (SDS) regulated under the REACH Regulation and sets requirements for packaging of hazardous chemicals.

There are significant hazard indicators for each hazard classification. All of them are shown in tables in parts 2 to 5 of the annex I of the CLP Regulation. Depending on the chemical's classification, there are a series of hazard statements (also called H statements) to indicate the specific risks/ hazards associated with each chemical. Each statement is codified according a letter (H for hazard and P for precaution) and a number with three figures. The hazard indicators are found in the CLP Regulation, but also in the safety data sheets regulated under the REACH Regulation. The CLP Regulation has its own chemical classification and it is different from the one shown for the Seveso III Directive (Royal Decree- law 840/2015). H statements from CLP Regulation need to be link with the annex I, parts 1 and 2 of the Seveso III Directive.

Summarizing, H statements can be taken from the safety data sheets for each chemical to participate in the polylactic acid production. Then, these statements can be related to annex I of Seveso III directive and, finally, the facility can be classified (if classifies).

12.2.2.1 Hazards of chemicals

Table 22. Definition of the hazards of the chemicals and correlation between CLP and Seveso III. (Own authorship).

Chemical substance	Pictogram	No. CAS	No. CE	CLP classification	Seveso III category
Lactic acid		79-33-4	201-196-2	H314 H315 H318 H290	Not applicable
Lactide		4511-42-6	224-832-0	H319	Not applicable
Water		7732-18-5	231-791-2	Not applicable	Not applicable
Poly (lactic acid)		9051-89-2	618-575-7	Not applicable	Not applicable

12.2.2.2 Indicators for hazards

The H statements with their codes and meanings found for the chemicals participating in the polylactic acid production are shown in table 23.

Table 23. Hazard indicator codes.

Hazard indicator codes	
H statements	**H statement meanings**
H314	Skin irritation/corrosion, categories 1A, 1B y 1C.
H315	Skin irritation/corrosion, category 2.
H318	Cause serious eye injury and eye irritation, category 1
H319	Cause serious eye injury and eye irritation, category 2.
H290	Corrosive to metals, category 1.

12.2.3 Classification according to Seveso III Directive

According to the Regulation CLP, previously-treated on this document on section 11.2.2, and for the purpose of adapting to a new classification system, the European Commission approves on 4 July, 2012, the 2012/18/UE Directive of the European Parliament and of the Council. This directive, which amends Directive 96/82/CE, will lead to the control of risks inherent to serious accidents involving hazardous substances. The Directive 2012/18/UE, also named as Seveso III, was incorporated to the Spanish legislation by the Royal-Decree 840/2015 of 21 September, approving the control measures of risks inherent to serious accidents involving hazardous substances. It is therefore, this royal-decree main objective is to prevent major accidents in where there are hazardous chemicals and limiting of their consequences.

In accordance with Royal-Decree 840/2015, many enterprises/facilities should indicate their degree of affectation in order to verify this royal-decree implementation. It is essential for the verification articles 2 and 3. The first article introduces the scope of the Royal-Decree 840/2015, while the second one, and includes some definitions of general interest. Some of the most highlighting definitions are: serious accident, hazard substance, establishment, upper-tier establishment and lower-tier establishment.

The degree of affectation should be determine taking into account, as first step, the relationship between the Seveso hazard categories and the CLP hazard indicators. The relationship can be established according to the aforementioned in section 11.2.2. Once the Seveso III hazard categories are known, the chemical substances can be classified as defined in the table columns of the parts 1 and 2 of annex I.

As shown in table 22, the substances of this project cannot not be classified according to Seveso III. For this reason, the facility has not an affectation degree and is not affected by Royal-Decree 840/2015.

12.3 Uncontrolled chemical reactivity study

12.3.1 Substances classification according to NFPA

NFPA 704, also named as Standard system for the identification of the hazards of materials for emergency response, is a standard which indicates the health, flammability, instability and other hazards of material under emergency conditions. This standard has been published by the

NFPA association (National Fire Protection Association) and provide a simple system for the understanding of the materials hazards. The main objectives of this standard are: provide necessary information for the public and staff safety, establishment of emergency plans and development of indicators for the evaluation of hazards by qualified personnel.

The evaluation system provided by NFPA allows for the hazards identification according to three main categories: health, flammability and instability. The degree of severity of each category is ranged between 0, for minimal hazard, and 4, for maximum hazard. The information is presented in a squared-on-point field which is commonly named as fire diamond. The square has four quadrant with different colours. Each category is related with one colour. In figure 36 is shown this relationship. [47]

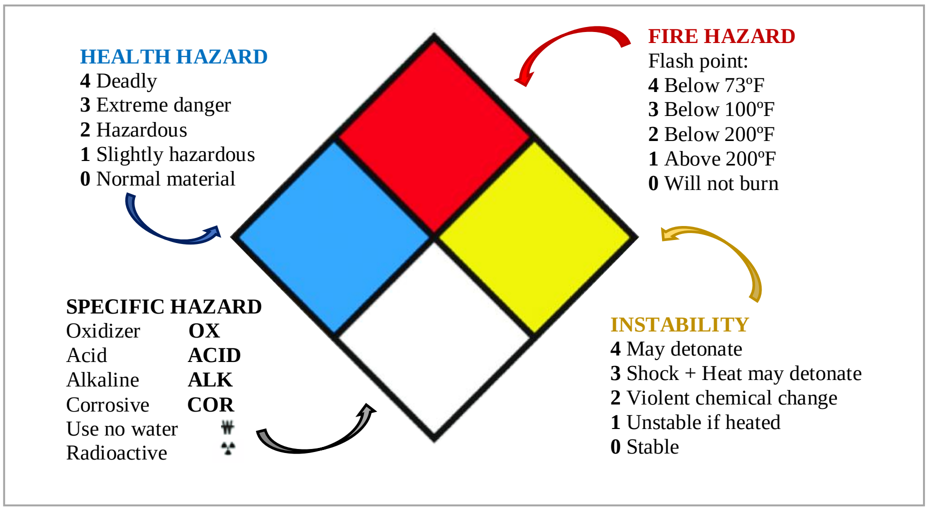


Figure 36. NFPA fire diamond for substance hazard classification. [48]

The severity of the hazards is slightly explained in figure 36. In addition to the three categories previously named there is a representation in white colour in the bottom quadrant of the fire diamond the special hazard indications.

The degree of hazard for each compound involve in the process explained in section 12.2.1 is shown in table 24. The hazard ratings ranged numerically as discuss before.

Table 24. NFPA 704 classification for the substances involve in this project. (Own authorship)

Substance	Flammability	Health	Instability reactivity	Special hazards
Poly (lactic acid)	1	1	0	None
Lactic acid	2	1	0	None
Lactide	1	0	0	None
Methanol	3	1	0	None
Dilactic acid	2	1	0	None
Water	0	0	0	None

12.3.2 Chemical compatibility and reactivity between substances

This chemical reactivity and compatibility study allows for the presentation of the main reactions taking place in the production process defined in this engineering project. There will be also an introduction to side reaction due to irregular operating conditions or due to the appearance of impurities in the system. Polymerization reactions are very complex and there can hardly be defined as a simple chemical reaction. Despite all of this, a summary of the reactivity will be outlined below.

Firstly, a polymer cannot be considered as a homogenous chemical product but should be seen as a mixture of several chemicals. The polymer consists of a combination of monomers of the initial reactive, lactic acid, and oligomers (dimers, trimmers, tetramer…) with very different molecular weights. The multiplicity of products contributes to its complexity.

The general reaction system for the poly (lactic acid) production process is summarized in figure 37.

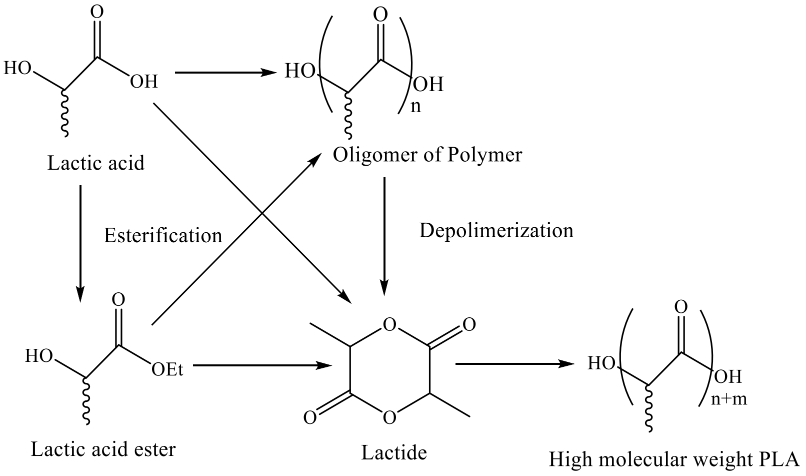


Figure 37. Main reactions and side reactions in the poly (lactic acid) production process. [49]

The lactic acid is a substance with a carboxylic group and an alcohol group. For this reason is a self-reacting component capable to polymerize in accordance to esterification exothermic reactions. This compound is soluble in water and dissociates to produce hydrogen and lactate ions. In agreement with the previously explained the pH of its solutions is acid.

Because of the carboxylic group and its solubility in water, the lactic acid may react with active metals with the production of hydrogen and metal salts. In other words, lactic acid is a substance with corrosive characteristics, for certain metals, which is relevant for the selection materials for the equipment of the process.

Lactic acid can also react with other impurities besides metals. Commercial lactic acid has sulphites traces, which may react with carboxylic acid in aqueous solution to produce heat and flammable/toxic gases.

Moreover, it reacts with alcohol impurities such as butanol, methanol, ethanol… Lactic acid can suffer exothermic esterification reactions in a temperature range of 130-250ºC in the presence of water and without any catalyst. However this impurities are in low proportion, so this side reactions takes place in lesser extent. In addition, lactic, which acts as intermediary in the poly (lactic acid) production, can be formed from esters generated by lactic acid. [50]

A reaction between the lactic acid carboxylic group and an alcohol is shown in figure 37.

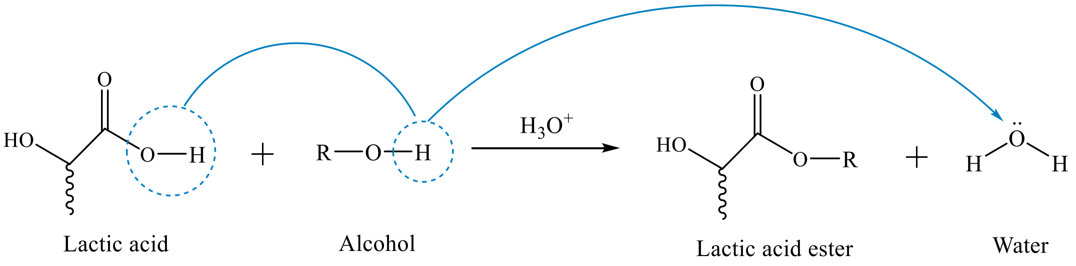


Figure 38. Lactic acid esterification with alcohols. (Own authorship)

The lactic acid has a low volatility and is thermally unstable. It reacts violently with alkalis and strong oxidizers with temperatures above 200ºC. Moreover, it can decompose in methanol and carbon dioxide above 260ºC as shown in equation 3.

$$CH_3CHOHCOOH \rightarrow CH_3CH_2OH + CO_2 \qquad (3)$$

A range of new possible side reactions like decarbonylation, decarboxylation and dehydration of lactic acid may appear during irregular operating conditions. These reactions occur above 450ºC and with high pressures. Some of them are compiled in figure 39.

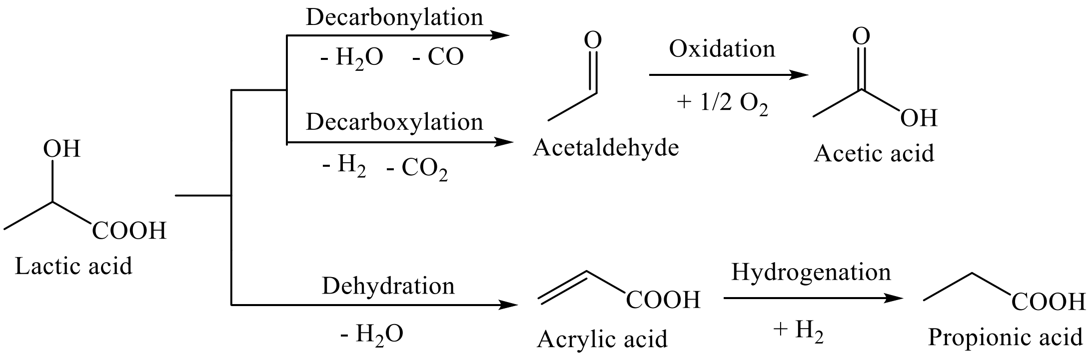


Figure 39. Reaction pathway of lactic acid at high temperatures and pressures. [51]

The poly (lactic acid) also participates in the reactive system because the nature of the reactions (reversible). This product suffers thermal degradation producing PLA molecules of lower molecular weight, lactic acid and cyclic oligomers. The degradation happens above 270ºC and the mechanisms are shown in figure 40.

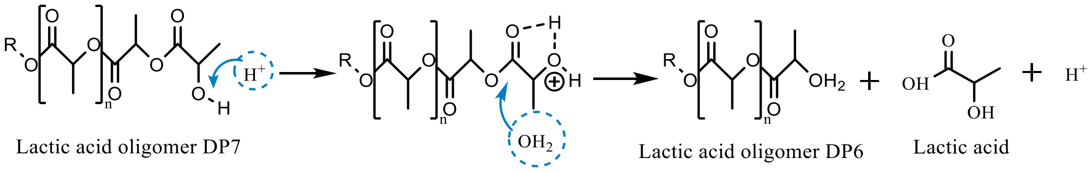


Figure 40. PLA thermal degradation mechanism in acidic media. [51]

12.4 Safety distances

The Center for Chemical Process safety (CCPS) in alliance with the American Institute of Chemical Engineers (AICHE) has recently published in 2018 some guidelines for siting and layout of facilities which provide guidance when selecting the location of the facility and when locating the equipment and process units. Regarding to the safety distances, special account must be taken to equipment with reactivity hazards and depending on the hazards the relative location of one piece of equipment with respect to another must be considered. The separation distances provided by the CCPS are for fire consequences and are based on historical data, which also includes codes and practices like GAP 2.5.2, GAP 2.5.2.A and PIP PNE00003. Table 25 shows the information provided by the CCPS guidelines. [52]

The final results of the distances are included in table 26.

Table 25. Safety distances for process equipment for fire consequences. [52]

DISTANCES	**Boundaries**		**Emergengy Equiment**				**Process Vessels /Equipment**			**Heat Transfer Equipment**					**Rotating Equipment**			**Transfer Equipment (Structures)**		
	(Another) Process Unit Battery Limit	Property	ESD Valves - Manual	Fire Pumps	Hydratants, Monitors	Water Spray & ESD Activation Switches	Equipment handling non-flammable, non- combustibl non-toxic materials	Reactors and desalters	(Another) Tower, Drum, Knock Out Pot, or In-process Storage Tank	Air cooled heat exchangers- process	Boilers, Air Compressors, Power generation (Utility Area)	(Another) Cooling Tower	Heat Exchangers	Fired Heaters, Cracking Furnaces	Gas Compressors, Expanders	Pumps handling Flammables (> autoignition or self-ignitiating)	Pumps handling Flammables (< autoignition or self-ignitiating)	Central Loading Racks for Trucks and Rail Cars	Liquefied Flammable Gas (LFG) Loading Racks for Trucks and Rail Cars	Main Pipe racks (piping not associated with unit)
Boundaries																				
Process Unit Battery Limit	30																			
Property	60																			
Emergency Equipment																				
ESD Valves- Manual	15	NM																		
Fire Pumps	75	NM	NM																	
Hydratants, Monitors	NM	NM	NM	NM																
Water Spray & ESD Activation Switches	15	NM	NM	NM	NM															
Process Vessels / Equipment																				
Equipment handling non-flammable, non-combustible, non-toxic materials	NA	NM	NM	NM	NM	NM														
Reactors and Desalters	NA	60	15	60	15	15	NM													
Towers, Drums, Knock Out Pots, In-Process Storage Tanks	NA	60	15	60	15	15	NM	8	8											
Heat Transfer Equipment																				
Air cooled heat exchangers - process	NA	60	15	60	15	15	NM	6	6											
Boilers, Air Compressors, Power Generation (Utility Area)	30	30	15	30	15	15	NM	30	30	30										
Cooling Towers	30	30	15	30	15	15	NM	30	30	30	30	15								
Heat Exchangers	NA	60	15	60	15	15	NM	8	8	5	30	30								
Fired Heaters, Cracking Furnaces	NA	60	15	60	15	15	NM	15	15	15	30	30	15							
Rotating Equipment																				
Gas Compressor, Expander	NA	60	15	60	15	15	NM	8	6	6	30	30	5	15						
Pumps handling Flammables (> autoignition or self-igniting materials)	NA	60	15	60	15	15	NM	5	5	5	30	30	5	15	5					
Pumps handling Flammables (< autoignition or self-igniting materials)	NA	60	15	60	15	15	NM	5	5	5	30	30	5	15	5	NM				
Transfer Equipment (Structures)																				
	75	30	15	60	15	15	NM	60	60	60	60	50	30	60	60	60	60			
Liquefied Flammable Gas (LFG) Loading Racks for Trucks and Rail Cars	75	110	15	75	15	15	NM	75	75	75	75	75	75	75	75	75	75	50		
Main Pipe Racks (piping not associated with unit)	NM	30	NM	15	NM	NM	NM	15	15	NM	15	15	5	15	15	15	15	15	15	
Process Pipe Racks	NM	60	NM	60	NM	NM	NM	5	5	NM	30	30	5	15	6	5	5	60	60	NM

Table 26. Results of the safety distances applied to the equipment of the process. (Own authorship)

	TK-101	P-101 A/B	E-101	P-102 A/B	E-102	V-101	E-103	R-201	P-201 A/B	V-301	E-301	P-301 A/B	R-301	P-302 A/B	E-302	T-401	E-401	E-402	V-401	P-401 A/B	V-402	E-403	T-402	E-404	V-403	P-402 A/B	V-404	P-403 A/B	E-405	T-403	E-406	E-407	P-404 A/B	V-405	P-405 A/B	E-408	R-501	P-501 A/B	R-502	P-502 A/B	X-601	E-601	V-601
TK-101	/																																											
P-101 A/B	5	/																																										
E-101	30	5	/																																									
P-102 A/B	5	/	5	/																																								
E-102	8	5	/	5	/																																							
V-101	8	5	8	5	8	/																																						
E-103	8	5	/	5	/	5	/																																					
R-201	8	5	8	5	8	8	8	/																																				
P-201 A/B	5	/	5	/	5	5	5	5	/																																			
V-301	8	5	8	5	8	8	8	8	5	/																																		
E-301	8	5	/	5	/	8	/	8	5	8	/																																	
P-301 A/B	5	/	5	/	5	5	5	5	/	5	5	/																																
R-301	8	5	8	5	8	8	8	/	5	8	8	5	/																															
P-302 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/																														
E-302	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/																													
T-401	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	/																												
E-401	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/	8	/																											
E-402	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/	8	8	/																										
V-401	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	/																									
P-401 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/	5	5	5	5	5	/																								
V-402	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	/																							
E-403	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/	8	/	/	8	5	8	/																						
T-402	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	/																					
E-404	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/	8	/	/	8	5	8	/	8	/																				
V-403	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	8	8	/																			
P-402 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/	5	5	5	5	5	/	5	5	5	5	5	/																		
V-404	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	8	8	8	5	/																	
P-403 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/	5	5	5	5	5	/	5	5	5	5	5	/	5	/																
E-405	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/	8	/	/	8	5	8	/	8	/	8	5	8	5	/															
T-403	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	8	8	8	5	8	5	8	/														
E-406	8	5	/	5	/	8	8	8	5	8	/	5	8	5	/	8	/	/	8	5	8	/	8	/	8	5	8	5	/	8	/													
E-407	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/	8	/	/	8	5	8	/	8	/	8	5	8	5	/	8	/	/												
P-404 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/	5	5	5	5	5	/	5	5	5	5	5	/	5	/	5	5	5	5	/											
V-405	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	8	8	8	5	8	5	8	8	8	8	5	/										
P-405 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/	5	5	5	5	5	/	5	5	5	5	5	/	5	/	5	5	5	5	/	5	/									
E-408	8	5	/	5	/	8	/	8	5	8	/	5	8	5	/	8	/	/	8	5	8	/	8	/	8	5	8	5	/	8	/	/	5	8	5	/								
R-501	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	8	8	8	5	8	5	8	8	8	8	5	8	5	8	/							
P-501 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/	5	5	5	5	5	/	5	5	5	5	5	/	5	/	5	5	5	5	/	5	/	5	8	/						
R-502	8	5	8	5	8	8	8	/	5	8	8	5	/	5	8	8	8	8	8	5	8	8	8	8	8	5	8	5	8	8	8	8	5	8	5	8	/	5	/					
P-502 A/B	5	/	5	/	5	5	5	5	/	5	5	/	5	/	5	5	5	5	5	/	5	5	5	5	5	/	5	/	5	5	5	5	/	5	/	5	5	/	5	/				
X-601	5	5	5	5	5	5	5	8	5	5	5	5	8	5	5	8	5	5	5	5	5	5	8	5	5	5	5	5	5	8	5	5	5	5	5	5	8	5	8	5	/			
E-601	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	8	8	8	5	8	5	8	8	8	8	5	8	5	8	8	5	8	5	8	/		
V-601	8	5	8	5	8	8	8	8	5	8	8	5	8	5	8	8	8	8	8	5	8	8	8	8	8	5	8	5	8	8	8	8	5	8	5	8	8	5	8	5	8	8	/

12.5 Relief systems

12.5.1 Relief valves

This project includes several relief valves for vacuum due to the operation at very low pressures. The sizing of the valves is a very important feature for the security system and all of them should be design. However, this project will only include the design of one of these valves. The sizing of the valve is performed with the API Recommended Practice 520.

Although the equipment to be design in these project is reactor R-502, this reactor is not the most significant equipment of the facility regarding to the control and protection for pressure.

Evaporator E-101 and reactor R-201 are equipment with strong requirements of vacuum for operation and have relief valves. Both are connected to steam jet ejectors. Failure in the vacuum system with the increase of motive steam in ejectors may sharply reduce the pressure, which decreases the elimination of impurities like water or methanol (which contributes to side reactions) and the final collapse of the equipment. For these reasons, the chosen valve is VSV-202.

The procedure for the relief valve design and the results obtained are explained in Annex II. Supporting calculations.

12.6 Elemental hazard analysis

There are different methodologies for the analysis of hazards during the design of a facility. Some of the most common are What-If Analysis, What-If/Checklist Analysis, HAZOP, HAZID and FMEA studies. All of them are qualitative hazard studies, but there are others, like the DOW index, which are quantitative.

The What-If Analysis was the hazard technique chosen for this project because its methodology allows for the hazard identification, the hazardous situation determination and the specification of the consequences of undesirable events in a simpler manner. This method can be consider as a basic step when performing more complex analysis for other methods, for example HAZOP.

This method generates questions and answers related to the poly (lactic acid) production process and more specifically, to reactor R-502 (the equipment design in detailed in this project). Although this method can be applied to the entire process, a more specific analysis has been considered.

Table 27. What-If Analysis worksheet for reactor R-502. (Own authorship)

What-If	Hazard	Consequence	Safeguards	Recommendation
Reactor R-502 experiences corrosion?	Weakening of the reactor materials.	Possible leak of reactants and utilities and equipment	Corrosion allowances and material selection during design.	Ensure appropriate material selection in agreement to materials properties.
Reactor R-502 losses cooling?	Temperature of the reactants too high.	Increase of the reaction rate and possible runaway.	Control Loop TIC/504 for temperature control	Installation of alarms for high temperature in control Loop TIC/504
Reactor R-502 is cooled too much?	Temperature of the reactants too low.	Unreacted lactide, product off-specifications and possible solidification of the polymer inside the reactor.	Control Loop TIC/504 for temperature control	Installation of alarms for low temperature in control Loop TIC/504
Reactor R-502 pressure is too low?	Decrease of the boiling point of lactide and materials resistance.	Possible formation of vapors of lactide and reduction of the conversion. For very low pressure the collapse of the reactor may occur.	Isolation of the equipment with valves in order to avoid reduction of pressure and safety relief valve VSV-502.	Other relieving devises may be installed in the equipment like rupture discs.
The reactor R-502 control fails?	Control system inoperative.	There is no capacity of reaction for possible changes in the process variables.	Protection for electric systems due to changes in voltage.	Improve maintenance of the control system.
The reactor R-502 coolant is leaking to the reactants?	The reactant mixture is contaminated	Poly (lactic acid) product off-specifications and the reactor could increase the pressure due to vaporization of water	Increasing of corrosion allowances for the reduction of possible leaks.	Improve the inherent design to avoid leaks.
The reactor R-502 is charge with too much catalyst?	Changes composition and viscosity of the final product	Increase of the polymer viscosity and very fast reaction with insufficiency in the heat removal.	Control Loop AIC/ 505 for the control of the composition.	Alarms for high composition should avoid dangerous excess of catalyst.

Table 28. What-If Analysis worksheet for reactor R-502 (Continuation). (Own authorship)

What-If	Hazard	Consequence	Safeguards	Recommendation
The Reactor R-502 leaks?	Contamination of the work area.	Losses of product and profits and environmental problems.	Increase corrosion and allowances. Increase also maintenance and check weld-joints.	Well-joints of category A with full radiography are recommended for the section of the reaction with more probability to leak.
The reactor R-502 is not clean?	Heat transfer risks	The overall heat transfer coefficient is sharply reduced due to fouling.	Ensure appropriate maintenance.	Verification and recording with a simple checklist the regular inspections and maintenance operations for the reactor.
The reactor R-502 flow rate in the tubes in increase?	Increase of the heat removal	Temperature reduction with unreacted lactide, product off-specifications and possible solidification of the polymer inside the reactor.	The control Loop TIC/504 has a control valve for the regulation of the cooling water flowing through the tube	Verify if the control valve has failed open.
One of the tubes of the reactor R-502 breaks?	The reactant mixture is contaminated	Poly (lactic acid) product off-specifications and the reactor could increase the pressure due to vaporization of water	Take into account the possibility of the tubes break during the design phase of the project.	Performed an exhaustive analysis of stresses in the tubes.
The composition in the shell of the reactor R-502 changes?	Possible increase or reduction of the viscosity	Very fast reaction with insufficiency in the heat removal and poly (lactic acid) off of specifications.	Control Loop AIC/ 505 for the control of the composition.	Check if the composition of the reactants includes other impurities than catalyst.
The reactor R-502 was not properly design?	Bad operation of the reactor in the required conditions	Insufficient heat removal, inadequate pressure drop, material corrosion.	Verification of the design for more than one engineer.	Verify if the design is in accordance with common standards.

Table 29. What-If Analysis worksheet for reactor R-502 (Continuation). (Own authorship)

What-If	Hazard	Consequence	Safeguards	Recommendation
The maintenance of reactor R-502 is not appropriate?	Fouling, mechanical failures, small breaches, …	Inappropriate operation and higher possibility of failure.	Verification and recording with a simple checklist the regular inspections and maintenance operations for the reactor.	Increase the budget for the maintenance of equipment.
The operation of reactor R-502 is opposite to normal operation?	Bad response of operators during emergencies.	Constant rectification of errors during operation and slow response when dangerous events show up.	Ensure the operators and other workers have received lessons for the new operation of the equipment.	Instruction manual should be available for the workers.
The emergency alarms of the control in reactor R-502 are not operative?	The operator of the control room does not detect when the process is out of normal operation.	Possible dangerous scenarios when variables are out of safety ranges.	The operator in the control room must take a look carefully to the most concerning variables.	Installation of alarms in the field.
The shell of reactor R-502 collapse?	Damages to operators and equipment.	New equipment costs.	Pressure and safety relief valve VSV-502.	Increase the thickness in the shell and installation of stiffening rings during design.

13. Instrumentation and control

13.1 Introduction

Nowadays, different control methods are used in the chemical industry to achieve a maximum efficiency during the manufacturing process and to fulfill with the objectives of industrial production. The control system will manipulate the main variables and will monitor the possible disturbances of a process in order to control them automatically, so an operator could guide the process until the product finally leaves the facility. The control system will compensate the changes in the variable with respect to a fixed operation conditions. Process control systems can apply to several sections of a plant and too many kind of equipment. Moreover, more than one variable can be controlled at the same time.

13.2 Process control system objectives

A control system is a group of components which has as basic objective the regulation of a desired value/variable regardless the external impacts in order to maintain a process within the specification limits. This value must be maintained at a reference value, which is also called set point. The value/variable must be controlled in order to fulfill with the following requirements: [53]

1. Safety in operation: This goal may include the environmental protection, the equipment protection and the human life protection. The control system takes action to ensure that the process is carried out within some safety constraints (maximum temperature, maximum pressure, etc.)
2. Smooth operation and production rate: The stability of the process is assured and the disturbances are practically suppressed.
3. Product quality and profit: Optimization of the production performance in order to maximize the difference between the profits from the sales and the costs from the facilities operation. The process is controlled to reduce the raw materials and utilities requirements so as to fulfill with the final specifications of the product.
4. Monitoring and diagnosis: The operator has constant information about the process operation and the equipment conditions with the minimal effort of data gathering. The production process is automatized.

13.3 Control system design

A subdivision of the facility in several categories must be considered when designing the control system of an entire chemical industrial facility, like the one propose for this project. Accordingly, the control system can be implemented for big equipment, for the main streams or for utilities. [54]

A control system can be described in agreement with the following strategy:

1. Identify the specific control objectives of the control loop.
2. Determine the input variables which may be manipulated or disturbances variables.
3. Determine the output variables which can be measured or unmeasured variables.
4. Identify all the constraints, classified as hard and soft.
5. Indicate the operating characteristics (continuous, batch or semicontinuous).
6. Explained all the considerations (environmental, safety, economics).
7. Specify the control structure.

13.4 Elements of a control loop

A control system consists of three main components: primary elements, controllers and final elements. Other components of the control loop are the transmission lines which transport the information from one component to another.

13.4.1 Primary elements

The primary elements are instruments or sensors capable of taking measures of the process variables. There are different types of primary elements available for industrial processes and they can be classified in accordance to the physical property to be measured. There are sensors for pressure, level, temperature flow rate, thermal conductivity, conductivity, moisture, etc. [55]

13.4.2 Controllers

The controllers are instruments capable of monitoring the process variable error because, when evaluating that error, they take corrective measures to reduce it and maintain a process variable in a predetermined value. For this reason, a controller accepts two signals: the set point signal and the actual process variable signal, which is recorded by the primary element.

The final response of the controller for the error correction is described as mode of control. There are different modes of control for a controller, which can be pure control or composite control modes. On-off, proportional, integral and derivatives are describes as pure control while proportional-integral, proportional-derivative and proportional-integral-derivative are composite control modes. [56]

- On-off operation: This is the cheapest control mode operation and is generally used when a rude control of the process is required. The final element of control switches the response from on to off or vice versa in agreement to the controller output.
- Proportional control: This mode of control can be defined mathematically as indicated in equation 4. This control mode removes fluctuations, although it has not a well response to steady state changes due to a constant error named offset.

$$V_{out} = K_p V_e \tag{4}$$

Where, V_{out} = Controller output signal, K_p =Gain of the controller, V_e =Error signal. The error signal is the difference between the voltage in the set point and in the variable of the process.

- Integral control: This control mode eliminates the error in the system because the output changes in a proportional magnitude and duration to the error signal. It is a continuous control, although has a slower response. This control mode can be expressed as indicated in equation 5.

$$\Delta V_{out} = K_i V_e \Delta t \tag{5}$$

  Where, V_{out} = Controller output signal, K_i = Integration constant, V_e =Error signal, Δt = Change of the time rate.

- Derivative control: This control mode responds to changes caused by an error signal when there is no steady-state error. Moreover, the respond has large oscillations. For all these reasons, this type of control mode is not used alone for the operation of a controller.

$$V_{out} = K_d \frac{\Delta V_e}{\Delta t} \tag{6}$$

  Where, V_{out} = Controller output signal, K_d = derivative gain, V_e =Error signal, Δt = Change of the time rate.

- Proportional-integral: This mode of control is capable of compensating the changes in the inputs and maintain the controlled variable in the set point.

$$V_{out} = K_p V_e + K_i \int V_e \, \Delta t \tag{7}$$

- Proportional- derivative control: This mode of control reduced the oscillations in the response and has a higher gain setting.

$$V_{out} = K_p V_e + \ K_d \frac{\Delta V_e}{\Delta t} \tag{8}$$

- Proportional-integral-derivative control: This mode of control combines the characteristics of the last three pure control modes. The proportional unit provides a fast response to disturbances, the integral unit has an output with a rate change proportional for a steady-state error and the derivative unit is responsible of the rate changes in the error signal.

$$V_{out} = K_p V_e + K_i \int V_e \, \Delta t + \; K_d \frac{\Delta V_e}{\Delta t} \tag{9}$$

13.4.3 Final elements

A final control element is an element of the control system with a clear influence on the process because modifies the variable of the process and reduces de variable error by means of an action. Valves are the most common final control elements although other equipment or instruments may act as a final elements of control.

13.5 Control loops - control strategies

A control loop is a segment of the control system of the process which manipulates a controlled parameter in order to maintain it in the set point. There are two main categories of control loops: basic control loops and advanced control loops. The basic control loops are only the simplest feedback loops. Feedforward control, cascade control, selective control, fuzzy control are examples of advanced control. This project will mainly consider the control explained below: [57]

- Feedback loop: This control loop is the most commonly used for process control. The process variable is measured and the information recorded is sent to a controller in order to compare the signal from the measured variable with the signal of the set point. The controller takes action and returns the process variable to the set point.

13.6 Symbology for the control systems

The control loops of a control system must be identified in agreement with the standard ISA S5.1 instrumentation symbol specification. Accordingly, each of the instruments of a control loop are designated with an alphanumeric code consisting of several letters and numbers. The first letter of the code indicates the type of measured variable and the second, the function of the control loop. The third letter can also indicate the function of the control loop or can be a modifier. The numbers of the control loop are the tag numbers, which indicates a particular control loop. The letters used during the design of the control loops for this project are shown in table 30. Some other symbology is also highlighted in tables 31, 32 and 33. [54]

Table 30. Nomenclature according to standard ISA-S5.1.

Letter	First letter		Succeeding letters		
	Measured or initiating variable	*Modifier*	*Readout or passive function*	*Output function*	*Modifier*
A	Analysis	-	Alarm	-	
C	User´s choice (Typically) Conductivity (electrical)	-	-	Control	Close
E	Voltage	-	Sensor (Primary element)	-	-
F	Flow rate	Ratio (fraction)	-	-	-
H	Hand	-	-	-	High
I	Current (electrical)	-	Indicate	-	-
L	Level	-	Light	-	Low
P	Pressure, vacuum	-	Point (test) connection	-	-
T	Temperature	-	-	Transmit	Through
V	Vibration, mechanical, analysis	-	-	Valve, damper, louver	-
Y	Event, state or presence	Y axis	-	Relay, compute, convert	-

Table 31. Elements of the control system. (Own authorship)

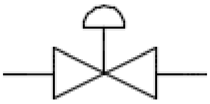
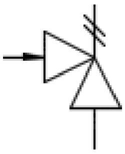
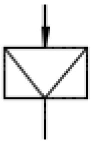
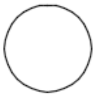
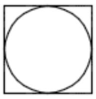
	Control valve with diaphragm actuator
	Generic gate valve
	Valve and drainage
	Vacuum relief valve
	Rupture disc for vacuum relief

Table 32. Instrument signals and line symbols. (Own authorship)

	Process line
	Electrical signal
	Pneumatic signal

Table 33. Accessibility of the instrument. (Own authorship)

	Field mounted, discrete instrument.
	Primary location accessible to operator, shared display and control.

13.7 Description of the control systems

13.7.1 Control loop for the process

13.7.1.1 Section 100: Lactic acid pre-pretreatment

Section 100 of the poly (lactic acid) production facility has 5 control loops which are described in tables 34 to 38. The control loops are: 102, 104, 105, 108 and 109. All these control loops maintain within appropriate operation conditions the equipment of these section.

Table 34. Control loop FIC/102 description. (Own authorship)

Control objective	Monitoring of the flow rate of lactic acid to be introduced in the process with the control of the output flow rate of tank TK-101.
Controlled variable	Output flow rate of the tank TK-101.
Manipulated variable	Output flow rate of the tank TK-101.
Principal element of control loop	Flow rate sensor FE/102. Flow rate transmitter FT/102. Flow rate indicating controller FIC/102. Pneumatic converter FY/102 Control valve FCV/104.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 35. Control loop TIC/104 description. (Own authorship)

Control objective	Monitoring of the temperature in the evaporator E-101 with temperature measurements in the liquid outlet stream of the equipment.
Controlled variable	Temperature in the liquid outlet stream of the evaporator E-101.
Manipulated variable	Flow rate of the low pressure steam utility inlet to evaporator E-101.
Principal element of control loop	Temperature sensor TE/104. Temperature transmitter TT/104. Temperature indicating controller TIC/104. Pneumatic converter TY/104. Control valve TCV/104.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 36. Control loop PIC/105 description. (Own authorship)

Control objective	Monitoring of the pressure inside the evaporator E-101 with measurements in the vapor outlet stream of the equipment.
Controlled variable	Pressure of the outlet stream of the evaporator E-101.
Manipulated variable	Flow rate of the high pressure steam utility of the ejector EJ-101.
Principal element of control loop	Pressure sensor PE/105. Pressure transmitter PT/105. Pressure indicating controller PIC/105. Pneumatic converter PY/105. Control valve PCV/105.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 37. Control loop LIC/108 description. (Own authorship)

Control objective	Monitoring of the liquid level for the vapor liquid phase separator V-101.
Controlled variable	Liquid level of the vapor phase separator V-101.
Manipulated variable	Flow rate of the outlet liquid stream (bottoms of the equipment) for vessel V-101.
Principal element of control loop	Level sensor LE/108. Level transmitter LT/108. Level indicating controller LIC/108. Pneumatic converter LY/108. Control valve LCV/108.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 38. Control loop PIC/109 description. (Own authorship)

Control objective	Monitoring of the pressure of the vapor outlet stream of the vapor-liquid phase separator V-101 in order to maintain the pressure inside the separator. The liquid-vapor equilibrium depends on the pressure inside the vessel.
Controlled variable	Pressure of the process vapor outlet stream of the separator V-101.
Manipulated variable	Flow rate of the process vapor outlet stream of the separator V-101.
Principal element of control loop	Pressure sensor PE/109. Pressure transmitter PT/109. Pressure indicating controller PIC/109. Pneumatic converter PY/109. Control valve PCV/109.
Control strategy	Feedback control.
Control algorithm	PID control.

13.7.1.2 Section 200: Pre-polymerization

Section 200 of the poly (lactic acid) production facility has 3 control loops which are described in tables 39 to 41. The considered control loops are: 201, 203 and 204.

Table 39. Control loop TIC/201 description. (Own authorship)

Control objective	Monitoring of the temperature in the reactor R-201with temperature measurements in the liquid outlet stream of the equipment.
Controlled variable	Temperature in the liquid outlet stream of the reactor R-201.
Manipulated variable	Flow rate of the cooling water supply to reactor R-201 required for refrigeration.
Principal element of control loop	Temperature sensor TE/201. Temperature transmitter TT/201. Temperature indicating controller TIC/201. Pneumatic converter TY/201. Control valve TCV/201.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 40. Control loop PIC/203 description. (Own authorship)

Control objective	Monitoring of the pressure inside the reactor R-201 with measurements in the vapor outlet stream of the equipment.
Controlled variable	Pressure of the outlet stream of the pre-polymerization reactor R-201.
Manipulated variable	Flow rate of the high pressure steam utility for ejector EJ-201.
Principal element of control loop	Pressure sensor PE/203. Pressure transmitter PT/203. Pressure indicating controller PIC/203. Pneumatic converter PY/203. Control valve PCV/203.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 41. Control loop PIC/204 description. (Own authorship)

Control objective	Monitoring of the pressure of vapor streams from the evaporator E-101 and reactor R-201. The control system in Ejector EJ-201 is needed for pressure controlled due to a low vacuum pressure in both, R-201 and E-101.
Controlled variable	Pressure of the vapor stream from EJ-201 and V-101.
Manipulated variable	Flow rate of the high pressure steam utility for ejector EJ-202.
Principal element of control loop	Pressure sensor PE/204. Pressure transmitter PT/204. Pressure indicating controller PIC/204. Pneumatic converter PY/204. Control valve PCV/204.
Control strategy	Feedback control.
Control algorithm	PID control.

13.7.1.3 Section 300: Lactide production

Section 300 of the poly (lactic acid) production facility has 3 control loops which are described in tables 42 to 44. The considered control loops are: 301, 306 and 308.

Table 42. Control loop TIC/301 description. (Own authorship)

Control objective	Monitoring of the temperature in the mixing vessel V-301 with temperature measurements in the outlet stream of the equipment.
Controlled variable	Temperature of the outlet stream of vessel V-301.
Manipulated variable	Flow rate of the cooling water supply needed for refrigeration of the equipment.
Principal element of control loop	Temperature sensor TE/301. Temperature transmitter TT/301. Temperature indicating controller TIC/301. Pneumatic converter TY/301. Control valve TCV/301.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 43. Control loop TIC/306 description. (Own authorship)

Control objective	Monitoring of the temperature in the reactor R-301 with temperature measurements in the liquid outlet stream of the equipment.
Controlled variable	Temperature of the liquid outlet stream of the reactor R-301.
Manipulated variable	Flow rate of the medium pressure steam needed for the heating of the process materials inside the equipment.
Principal element of control loop	Temperature sensor TE/306. Temperature transmitter TT/306. Temperature indicating controller TIC/306. Pneumatic converter TY/306. Control valve TCV/306.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 44. Control loop PIC/308 description. (Own authorship)

Control objective	Monitoring of the pressure inside the reactor R-301 with measurements in the vapor outlet stream of the equipment.
Controlled variable	Pressure of the outlet stream of the reactor R-301.
Manipulated variable	Flow rate of the high pressure steam utility of the ejector EJ-301.
Principal element of control loop	Pressure sensor PE/308. Pressure transmitter PT/308. Pressure indicating controller PIC/308. Pneumatic converter PY/308. Control valve PCV/308.
Control strategy	Feedback control.
Control algorithm	PID control.

13.7.1.4 Section 400: Lactide purification

Section 400 of the poly (lactic acid) production facility has 21 control loops which are described in tables 45 to 65. The considered control loops are: 401, 402, 403, 407, 409, 412, 413, 414, 415, 419, 420, 421, 424, 425, 427, 428, 429, 430, 433 and 434.

Table 45. Control loop FIC/401 description. (Own authorship)

Control objective	Monitoring of the flow rate of the liquid stream distillate to be reflux to column T-401 in agreement to the reflux ratio required for operation.
Controlled variable	Flow rate of the reflux stream in column T-401.
Manipulated variable	Flow rate of the reflux stream in column T-401.
Principal element of control loop	Flow rate sensor FE/401. Flow rate transmitter FT/401. Flow rate indicating controller FIC/401. Pneumatic converter FY/401. Control valve FCV/401.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 46. Control loop LIC/402 description. (Own authorship)

Control objective	Monitoring of the liquid level in the bottoms of the column T-401 in order to avoid flooding.
Controlled variable	Liquid level in the bottoms of the column T-401.
Manipulated variable	Flow rate of the liquid bottoms product of column T-401.
Principal element of control loop	Level sensor LE/402. Level transmitter LT/402. Level indicating controller LIC/402. Pneumatic converter LY/402. Control valve LCV/402.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 47. Control loop TIC/403 description. (Own authorship)

Control objective	Monitoring of the temperature in the bottoms of the column T-401 to fulfill with operation requirements (temperature for separation of the components).
Controlled variable	Temperature bottoms of the column T-401.
Manipulated variable	Flow rate of the input heating utility in the reboiler E-402.
Principal element of control loop	Temperature sensor TE/403. Temperature transmitter TT/403. Temperature indicating controller TIC/403. Pneumatic converter TY/403. Control valve TCV/403.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 48. Control loop LIC/407 description. (Own authorship)

Control objective	Monitoring of the liquid level in the bottoms of the vapor-liquid phase separator vessel V-401.
Controlled variable	Liquid level in the V-401
Manipulated variable	Flow rate liquid stream outlet of V-401.
Principal element of control loop	Level sensor LE/407. Level transmitter LT/407. Level indicating controller LIC/407. Pneumatic converter LY/407. Control valve LCV/407.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 49. Control loop PIC/408 description. (Own authorship)

Control objective	Monitoring of the pressure of the vapor outlet stream of the vapor-liquid phase separator V-401 in order to maintain the pressure inside the separator. The liquid-vapor equilibrium depends on the pressure inside the vessel.
Controlled variable	Pressure of the outlet process stream of the separator V-401.
Manipulated variable	Flow rate of the outlet process stream of the separator V-401.
Principal element of control loop	Pressure sensor PE/408. Pressure transmitter PT/408. Pressure indicating controller PIC/408. Pneumatic converter PY/408. Control valve PCV/408.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 50. Control loop PIC/409 description. (Own authorship)

Control objective	Monitoring of pressure inside the column T-401 in order to maintain a constant vacuum.
Controlled variable	Pressure of the vapor stream leaving the top of the column T-401.
Manipulated variable	Flow rate of the high pressure steam utility required for ejector EJ-401.
Principal element of control loop	Pressure sensor PE/409. Pressure transmitter PT/409. Pressure indicating controller PIC/409. Pneumatic converter PY/409. Control valve PCV/409.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 51. Control loop PIC/412 description. (Own authorship)

Control objective	Monitoring of the pressure of the vapor stream from the vapor liquid phase separator V-402. The control system in Ejector EJ-402 is needed for pressure controlled due to a low vacuum pressure in column T-401.
Controlled variable	Pressure in the vapor outlet of the vessel V-402.
Manipulated variable	Flow rate of the high pressure steam utility required for ejector EJ-402.
Principal element of control loop	Pressure sensor PE/412. Pressure transmitter PT/412. Pressure indicating controller PIC/412. Pneumatic converter PY/412. Control valve PCV/412.
Control strategy	Feedback control.
Control algorithm	PID control.

As the operation of the column T-401 is similar to the column T-402, the control loops required for the process control of the lactide purification in column T-402 are analogous to those of the column T-401. For such reason, the explanation of the control loops LIC/401, LIC/402, TIC/403, LIC/407, PIC/408, PIC/409 and PIC/412 is similar to the FIC/413, LIC/414, TIC/415, LIC/419, PIC/420, PIC/421 and PIC/424, respectively.

Table 52. Control loop FIC/413 description. (Own authorship)

Control objective	Monitoring of the flow rate of the liquid stream distillate to be reflux to column T-402 in agreement to the reflux ratio required for operation.
Controlled variable	Flow rate of the reflux stream in column T-402.
Manipulated variable	Flow rate of the reflux stream in column T-402.
Principal element of control loop	Flow rate sensor FE/413. Flow rate transmitter FT/413. Flow rate indicating controller FIC/413. Pneumatic converter FY/413. Control valve FCV/413.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 53. Control loop LIC/414 description. (Own authorship)

Control objective	Monitoring of the liquid level in the bottoms of the column T-402 in order to avoid flooding.
Controlled variable	Liquid level in the bottoms of the column T-402.
Manipulated variable	Flow rate of the liquid bottoms product of column T-402.
Principal element of control loop	Level sensor LE/414. Level transmitter LT/414. Level indicating controller LIC/414. Pneumatic converter LY/414. Control valve LCV/414.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 54. Control loop TIC/415 description. (Own authorship)

Control objective	Monitoring of the temperature in the bottoms of the column T-402 to fulfill with operation requirements (temperature for separation of the components).
Controlled variable	Temperature bottoms of the column T-402.
Manipulated variable	Flow rate of the input heating utility in the reboiler E-405.
Principal element of control loop	Temperature sensor TE/415. Temperature transmitter TT/415. Temperature indicating controller TIC/415. Pneumatic converter TY/415. Control valve TCV/415.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 55. Control loop LIC/419 description. (Own authorship)

Control objective	Monitoring of the liquid level in the bottoms of the vapor-liquid phase separator vessel V-403.
Controlled variable	Liquid level in the V-403.
Manipulated variable	Flow rate liquid stream outlet of V-403.
Principal element of control loop	Level sensor LE/419. Level transmitter LT/419. Level indicating controller LIC/419. Pneumatic converter LY/419. Control valve LCV/419.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 56. Control loop PIC/420 description. (Own authorship)

Control objective	Monitoring of the pressure of the vapor outlet stream of the vapor-liquid phase separator V-403 in order to maintain the pressure inside the separator. The liquid-vapor equilibrium depends on the pressure inside the vessel.
Controlled variable	Pressure of the vapor outlet stream of the separator V-403.
Manipulated variable	Flow rate of the vapor outlet stream of the separator V-403.
Principal element of control loop	Pressure sensor PE/420. Pressure transmitter PT/420. Pressure indicating controller PIC/420. Pneumatic converter PY/420. Control valve PCV/420.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 57. Control loop PIC/421 description. (Own authorship)

Control objective	Monitoring of pressure inside the column T-402 in order to maintain a constant vacuum.
Controlled variable	Pressure of the vapor stream leaving the top of the column T-402.
Manipulated variable	Flow rate of the high pressure steam utility required for ejector EJ-403.
Principal element of control loop	Pressure sensor PE/421. Pressure transmitter PT/421. Pressure indicating controller PIC/421. Pneumatic converter PY/421. Control valve PCV/421.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 58. Control loop PIC/424 description. (Own authorship)

Control objective	Monitoring of the pressure of the vapor stream from the vapor liquid phase separator V-402. The control system in Ejector EJ-404 is needed for pressure controlled due to a low vacuum pressure in column T-401.
Controlled variable	Pressure in the vapor outlet of the vessel V-402.
Manipulated variable	Flow rate of the high pressure steam utility required for ejector EJ-404.
Principal element of control loop	Pressure sensor PE/424. Pressure transmitter PT/424. Pressure indicating controller PIC/424. Pneumatic converter PY/424. Control valve PCV/424.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 59. Control loop TIC/425 description. (Own authorship)

Control objective	Monitoring of the temperature of the feeding to the column T-403. The process stream must be cooled until reached the established set point (inlet temperature to column T-403).
Controlled variable	Temperature of the feeding stream to column T-403
Manipulated variable	Inlet flow rate of the cooling water supply utility in heat exchanger E-407.
Principal element of control loop	Temperature sensor TE/425. Temperature transmitter TT/425. Temperature indicating controller TIC/425. Pneumatic converter TY/425. Control valve TCV/425.
Control strategy	Feedback control.
Control algorithm	PID control.

Finally the control system for column T-403 is for the control loops in tables 60 to 65.

Table 60. Control loop PIC/427 description. (Own authorship)

Control objective	Monitoring of the vacuum pressure inside the column.
Controlled variable	Pressure of the vapor stream leaving the top of the column T-403.
Manipulated variable	Flow rate of the high pressure steam utility required for ejector EJ-405.
Principal element of control loop	Pressure sensor PE/427. Pressure transmitter PT/427. Pressure indicating controller PIC/427. Pneumatic converter PY/427. Control valve PCV/427.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 61. Control loop TIC/428 description. (Own authorship)

Control objective	Monitoring of the temperature in the bottoms of the column T-403 to fulfill with operation requirements (temperature for separation of the components).
Controlled variable	Temperature bottoms of the column T-403.
Manipulated variable	Flow rate of the input heating utility in the reboiler E-409.
Principal element of control loop	Temperature sensor TE/428. Temperature transmitter TT/428. Temperature indicating controller TIC/428. Pneumatic converter TY/428. Control valve TCV/428.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 62. Control loop LIC/429 description. (Own authorship)

Control objective	Monitoring of the liquid level in the bottoms of the column T-403 in order to avoid flooding.
Controlled variable	Liquid level in the bottoms of the column T-403.
Manipulated variable	Flow rate of the liquid bottoms product of column T-403.
Principal element of control loop	Level sensor LE/429. Level transmitter LT/429. Level indicating controller LIC/429. Pneumatic converter LY/429. Control valve LCV/429.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 63. Control loop FIC/430 description. (Own authorship)

Control objective	Monitoring of the flow rate of the liquid stream distillate to be reflux to column T-403 in agreement to the reflux ratio required for operation.
Controlled variable	Flow rate of the reflux stream in column T-403.
Manipulated variable	Flow rate of the reflux stream in column T-403.
Principal element of control loop	Flow rate sensor FE/430. Flow rate transmitter FT/430. Flow rate indicating controller FIC/430. Pneumatic converter FY/430. Control valve FCV/430.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 64. Control loop PIC/433 description. (Own authorship)

Control objective	Monitoring of the pressure stream in the column T-403. The control system in Ejector EJ-406 is needed for pressure controlled due to a low vacuum pressure in column T-403.
Controlled variable	Pressure in the vapor outlet of the ejector EJ-405.
Manipulated variable	Flow rate of the high pressure steam utility required for ejector EJ-406.
Principal element of control loop	Pressure sensor PE/433. Pressure transmitter PT/433. Pressure indicating controller PIC/433. Pneumatic converter PY/433. Control valve PCV/433.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 65. Control loop LIC/434 description. (Own authorship)

Control objective	Monitoring of the liquid level in the bottoms of the vessel drum V-405.
Controlled variable	Liquid level in V-405.
Manipulated variable	Flow rate of the liquid stream outlet (distillate) of V-405.
Principal element of control loop	Level sensor LE/434. Level transmitter LT/434. Level indicating controller LIC/434. Pneumatic converter LY/434. Control valve LCV/434.
Control strategy	Feedback control.
Control algorithm	PID control.

13.7.1.5 Section 500: Polymerization reaction system

Section 200 of the poly (lactic acid) production facility has 3 control loops which are described in tables 66 to 68. The considered control loops are: 501, 504 and 505.

Table 66. Control loop TIC/501 description. (Own authorship)

Control objective	Monitoring of the reactor temperature in order to achieve a good refrigeration and avoid a possible runaway during the polymerization reaction in reactor R-501.
Controlled variable	Temperature of the outlet process stream of the reactor R-501.
Manipulated variable	Inlet flow rate of the cooling water supply utility required for reactor R-501.
Principal element of control loop	Temperature sensor TE/501. Temperature transmitter TT/501. Temperature indicating controller TIC/501. Pneumatic converter TY/501. Control valve TCV/501.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 67. Control loop TIC/504 description. (Own authorship)

Control objective	Monitoring of the reactor temperature in order to achieve a good refrigeration and avoid a possible runaway during the polymerization reaction in reactor R-502.
Controlled variable	Temperature of the outlet process stream of the reactor R-502.
Manipulated variable	Inlet flow rate of the cooling water supply utility required for reactor R-502.
Principal element of control loop	Temperature sensor TE/504. Temperature transmitter TT/504. Temperature indicating controller TIC/504. High temperature alarm TAH/504. Low temperature alarm LAH/504. Pneumatic converter TY/504. Control valve TCV/504.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 68. Control loop AIC/505 description. (Own authorship)

Control objective	Monitoring of the composition in reactor R-502. The viscosity and the molecular weight of the final polymer must be controlled in order to avoid high pressure drops inside the reactor due to high viscosity and to achieve a good quality product.
Controlled variable	The composition of the outlet process stream in reactor R-502.
Manipulated variable	Flow rate of the inlet stream (catalyst 2) which is a mixture of the catalyst and co-catalyst.
Principal element of control loop	Temperature sensor TE/505. Temperature transmitter TT/505. Temperature indicating controller TIC/505. High composition alarm AAH/504. Low composition alarm AAL/504. Pneumatic converter TY/505. Control valve TCV/505.
Control strategy	Feedback control.
Control algorithm	PID control.

13.7.1.6 Section 600: Volatilization

Section 200 of the poly (lactic acid) production facility has 2 control loops which are described in tables 69 and 70. The considered control loops are: 603 and 604.

Table 69. Control loop PIC/603 description. (Own authorship)

Control objective	Monitoring of the pressure in order to maintain the vacuum pressure required for volatilization operations.
Controlled variable	Pressure in the vapor outlet process stream of the equipment V-601.
Manipulated variable	Flow rate of the high pressure steam utility needed in ejector EJ-601.
Principal element of control loop	Pressure sensor PE/603. Pressure transmitter PT/603. Pressure indicating controller PIC/603. Pneumatic converter PY/603. Control valve PCV/603.
Control strategy	Feedback control.
Control algorithm	PID control.

Table 70. Control loop LIC/604 description. (Own authorship)

Control objective	Monitoring of the liquid level in the bottoms of the vapor-liquid phase separator V-601.
Controlled variable	Liquid level in separator V-601.
Manipulated variable	Flow rate of the liquid outlet stream of the separator V-601.
Principal element of control loop	Level sensor LE/604. Level transmitter LT/604. Level indicating controller LIC/604. Pneumatic converter LY/604. Control valve LCV/604.
Control strategy	Feedback control.
Control algorithm	PID control.

13.7.2 Alarms, indicators and relieving devises

13.7.2.1 Alarms

The alarms are systems installed along the facilities with the main goal to warn the operator of an event when the process parameter are out of normal conditions. These parameters could be over or under the alarm triggering point. The alarms considered in the facility to be design are: LAH/101, LAL/101, TAH/504, TAL/504, AAH/505 and AAL/505.

All of them are alarms handle through BPCS (Basic Process Control System) and they can be categorized as stand-alone alarms and alarms as part of other parameter monitoring instruments. LAH/101 and LAL/101 are included in the second category, while the rest of the previously mentioned alarms belong to the first one.

Alarm LAH/101 prevents loss of containment and alarm LAL/101 prevents the tank TK-101 to be completely discharge.

Alarms TAH/504 and TAL/504 warns about high and low temperature of operation in reactor R-502. The first alarm is especially important to prevent possible runaways.

Alarms AAH/505 and AAL/505 indicates high and low composition in the polymer product obtained in the reactor R-502 of the catalyst/co-catalyst mixture, which has a strong influence on the viscosity and molecular weight of the polymer.

13.7.2.2 Indicators

The indicators are instruments with the capability of taking measures of the operation parameters. Most of the indicators considered in this production process are indicators installed in the field and are used as a parameter indicator for the operator in the field. These two parameters to be measured are the flow rate and the temperature. The flow rate field indicators are: FI/107, FI/110, FI/304, FI/309, FI/405, FI/428, FI/410, FI/417, FI/422, FI435 and FI/601. The temperature field indicators are: TI/106, TI/111, TI/305, TI/110, TI/406, TI/411, TI/418, TI/423, TI/436 and TI/602.

The indicators located in the main panel are: LIC/101 and AIC/303.

13.7.2.3 Relieving devises

The relieving devises, which are one of the last resource for the protection of an industrial facility, are a viable solution against overpressure and under pressure situations which may cause dangerous scenarios. As the entire process for the production of poly (lactic acid) is under vacuum pressure conditions, the relieving devises are safety valves and rupture discs. More specifically, VRDs (vacuum relief devises) and vacuum rupture discs.

The VRDs for this project are: VSV/103, VSV/202, VSV/302, VSV/503 and VSV/502.

The vacuum rupture discs are: VSE/307, VSE/404, VSE/416 and VSE/426.

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ANNEX I

Mass and Energy balances

Index

1. Mass balances

1.1 Mass balance on the overall process

A material balance is the implementation of the mass conservation statement to process operation systems. The main goal is the description of the material quantities passing through the system. A system can be defined as the studied space volume. For a global material balance the system is the entire production process.

A general mass balance for the overall process where the mass is conserved can be written as:

$$Accumulation = (input - output) \quad (1)$$

Where,

Accumulation = Material quantity charge inside the system.

Input = Material entering the system by crossing the system boundary.

Output = Material leaving the system by crossing the system boundary.

Two types of balances (with or without accumulation) can be recognized depending on the process classification. The processes in question can be: batch, continuous, semi-batch, steady state and transient state. The poly (lactic acid) production process operates continuously at steady state manufacturing 50,000 tons of the final product in 330 days of operation during 24 hours.

As there is not accumulation, all materials entering the process are leaving the process (input is equal to the output).

Mass balances for individual substances where there are chemical reactions can be written as:

$$Accumulation = (input - output) + (generation - consumption) \quad (2)$$

Where,

Generation = Material produced by chemical reaction within the system.

Consumption =Material used by chemical reaction within the system.

As there is no accumulation, just like in the general balance, this term is considered to be zero in equation 2.

All mass balances can be solved by taking into account the following procedure:

1. Analysis of the information and set the goal of the mass balance.
2. Segregation and determination of all known quantities and unknown quantities for the streams of the process.
3. Choosing of calculation bases. (optional, if needed)

4. Delimitation of the system boundaries.
5. Determination of the unknowns and the number of equations.
6. Calculation of the unknowns. [1]

Table 1. Mass balance of the overall process results. (Own authorship)

	INPUT	**OUTPUT**
Mass flows (kg/h)		
L-Lactic acid	9857.74	586.05
D-Lactic acid	518.83	35.04
Water	2205.02	4156.06
Volatile impurities	388.91	388.91
Non-volatile impurities	0.21	0.21
Poly (lactic acid)	0	5873.27
L-Lactide	0	693.60
D-Lactide	0	74.93
Meso-Lactide	0	775.04
Oligomers	0	387.69
Catalyst 1	1.00	1.00
Stabilizer 1	0.20	0.20
Catalyst 2	7.85	7.74
Deactivating Agent	9.22E-04	9.22E-04
Stabilizer 2	0.50	0.50
Total mass flows (kg/h)	**12980.26**	**12980.26**
Closure	0.00%	

1.2 Mass balance by equipment

The PLA production process can be considered as a multiunit process because consists on more than one-unit operation or equipment. For this reason, the material balances are solved through the definition of subsystems delimited by boundaries. These subsystems usually encompass equipment units. According to this explanation and the clarification for systems in section 1.1 of the Annex I: Mass and Energy balances, equation 2 can be applied for mass balances in equipment. In this section a detailed description of the mass balances is shown for equipment whose input and output streams presents different material quantities. This is the case of mass separation equipment and reactors. Mass transfer equipment is not included in this annex, so as the facility utilities. [1]

1.2.1 Evaporator E-101

The mass balance in the evaporator has been performed taking into account a vapor-liquid equilibrium and its operating mode. The lactic acid solution entering the separation chamber of the evaporator is a two-phase mixture with lactic acid, water, volatile impurities and non-volatile impurities. The volatile impurities are assumed to be methanol, which is one on the greatest impurities in lactic acid with water.

For a pressure of 6.5 kPa and a temperature of 95ºC, there are different distribution coefficients for each compound. The lactic acid, water and methanol (volatile impurities) Ki values are 0.048, 12.998 and 46.228, respectively. The vapor liquid equilibrium provides information about the total amount of the feed remaining as liquid or vapor and the composition in the liquid and the vapor. The liquid feed evaporates and a 76.99% remains liquid during the evaporation process.

Table 2. Mass balance results in the evaporator E-101. (Own authorship)

STREAM	2	3	4
Mass flows (kg/h)			
L-Lactic acid	9857.74	510.36	9347.37
D-Lactic acid	518.83	26.86	491.97
Water	2205.02	2065.30	139.72
Volatile impurities	388.91	381.65	7.26
Non-volatile impurities	0.21	0	0.21
Total mass flows (kg/h)	**12970.71**	**2984.18**	**9986.53**

1.2.2 Pre-polymerization reactor R-201

The mass balance in the pre-polymer reactor was calculated considering first the following assumptions:

1. The reactivity in this reactor consists of one ideal reaction with equal stoichiometry.
2. The stoichiometry of the reaction is not settled and depends on the molecular weight of the polymer, however for a high molecular weight polymer the stoichiometry between the lactic acid and the water is 1:1.
3. The reactivity does not depend on the chain length of the polymer.
4. The considered reaction is not reversible because the by-product is continuously removed.
5. The lactide ring is not formed in this reactor.
6. The average molecular weight of the final polymer is 2500 g/mol and the polydispersity is low.
7. Lactic acid does not evaporate because of its boiling point (186.31ºC at 35 kPa), its low vapor pressure and the mass transfer resistance in liquid phase due to the formation of the polymer.
8. Volatile impurities are completely removed with the outlet vapor stream.

9. A catalyst and co-catalyst is not required.

The chemical reaction for this reactor can be represented as shown in equation 3. [2].This reaction represents the step-growth polymerization for lactic acid.

$$(AB)_n + (AB)_m \rightarrow (AB)_{n+m} + W \tag{3}$$

Where,

$(AB)_n$= Oligomer or polymer of lactic acid with n units of monomer.

$(AB)_m$ = Oligomer or polymer of lactic acid with m units of monomer.

W = Representation of the by-product, water.

The conversion of the monomer (lactic acid) has considered to be 0,943 and is shown in equation 4 as p. The dispersity index or DI, which maximum value is 2, indicates that for the selected conversion, the polymer is quite homogeneous, as assumed before.

$$PDI = 1 + p \tag{4}$$

The water to be removed as vapor was calculated in agreement with the equation 5 and is the sum of the free water remaining in lactic acid solution and the water formed during the polymerization. The degree of polymerization needed for the calculation of equation 5 is 17.35 and is calculated according equation 6. [3]

$$RW = \left[1 - \frac{M_{H_2O}}{\overline{PD}\left(M_{H_2O} - M_{LA} + \frac{M_{LA}}{x_{LA}}\right)}\right] \tag{5}$$

Where,

M_{H_2O}= Molecular weight of water.

M_{LA} =Molecular weight of lactic acid.

x_{LA} = Mass fraction of lactic acid in solution.

PD = Degree of polymerization.

$$\overline{PD} = \frac{\overline{M_n} - M_{H_2O}}{M_{LAU}} \tag{6}$$

Where,

M_{LAU} = Molecular weight of lactic acid unit.

$\overline{M_n}$ = Number average molar mass.

Table 3. Mass balance results in the pre-polymerization reactor R-201. (Own authorship).

STREAM	10	11	12
Mass flows (kg/h)			
L-Lactic acid	9347.37	0	504.57
D-Lactic acid	491.97	0	54.51
Water	139.72	1888.70	107.03
Volatile impurities	7.26	7.26	0
Non-volatile impurities	0.21	0	0.21
Poly (lactic acid)	0	0	7424.26
Total mass flows (kg/h)	**9986.53**	**1895.96**	**8090.57**

1.2.3 Depolymerization reactor R-301, purge and mixer tank V-301

The catalyst has an important role in the conversion of low molecular weight poly (lactic acid) to lactide. According to some bibliography data, the % crude lactide in product using stannous octoate catalyst is around 75% and the crude lactide is a mixture of lactic acid dimer, lactic acid monomer, water and lactide. The lactide yield value taken is 91.5% and the D,L-lactide fraction is 88,5%. [4]

Keeping with this, the crude lactide formed in the depolymerization reactor can be estimated as shown in equations 7, 8, and 9.

$$\%Crude\ lactide\ in\ product = \frac{Amount\ of\ crude\ lactide\ produced}{Amount\ of\ PLA\ charged\ in\ the\ reactor}\ 100\ (\%) \tag{7}$$

$$Lactide\ yield = \frac{Amount\ of\ Lactide\ (D,L-and\ meso-lactide)\ produced}{Amount\ of\ crude\ lactide\ produced}\ 100\ (\%) \tag{8}$$

$$D,L-lactide\ fraction = \frac{Amount\ of\ D,L-lactide\ produced}{Amount\ of\ Lactide\ (D,L-and\ meso-lactide)\ produced}\ 100\ (\%) \tag{9}$$

Moreover, a side reaction was considered in this reactor: a polycondensation similar to the one explained for the pre-polymerization reactor. The conversion of the lactic acid monomer in this case is 0.85 and the product of this reaction is mainly very short length chain polymer (lactic acid dimer).

Table 4. Mass balance results in the depolymerization reactor R-301. (Own authorship)

STREAM	22	23	24
Mass flows (kg/h)			
L-Lactic acid	504.57	75.69	0
D-Lactic acid	54.51	8.18	0
Water	107.03	202.07	0
Volatile impurities	0	0	0
Non-volatile impurities	4.15	0	4.15
Poly (lactic acid)	10566.64	0	3307.76
L-Lactide	0	5793.36	0
D-Lactide	0	625.88	0
Meso-Lactide	0	832.12	0
Oligomers	0	387.69	0
Catalyst 1	20.00	0	20.00
Stabilizer 1	4.00	0	4.00
Total mass flows (kg/h)	**11260.89**	**7924.98**	**3335.91**

However, the mass balance in the depolymerization reactor R-301 cannot be calculated without taking into account the stirrer storage tank and the purge. This is one example of a multiunit process calculation for the mass balance. The results already shown in table 4 were calculated taking into account this assumption. Results for the stirrer storage tank and the purge are shown in table 5.

Table 5. Mass balance results for the purge and V-301. (Own authorship)

STREAM	16	18	19	20	17	26
Mass flows (kg/h)						
L-Lactic acid	504.57	0	0	504.57	0	0
D-Lactic acid	54.51	0	0	54.51	0	0
Water	107.03	0	0	107.03	0	0
Volatile impurities	0.00	0	0	0.00	0	0
Non-volatile impurities	0.21	0	0	4.15	4	0
Poly (lactic acid)	7424.26	0	0	10566.64	3142	165
L-Lactide	0	0	0	0	0	0
D-Lactide	0	0	0	0	0	0
Meso-Lactide	0	0	0	0	0	0
Oligomers	0	0	0	0	0	0
Catalyst 1	0	1.0	0	20.00	19	1
Stabilizer 1	0	0	0.20	4.00	4	0
Total mass flows (kg/h)	**8090.57**	**1.00**	**0.20**	**11260.89**	**3169.12**	**166.80**

1.2.4 Column T-401

The mass balances in column T-401 were solved taking into account a multicomponent separation and a mixed condenser. The feed to the column is completely specified, so as the pressure in the column. For multicomponent distillation the key components must be specified. The heavy key component (HK) is lactide and the light key component (LK) is lactic acid. Dilactic acid and water are light non key components. At 2 kPa and 112 ºC the relative volatilities of each component, so as the distribution coefficients are shown in table 6.

Table 6. Relative volatilities and distribution coefficients. (Own authorship)

Component	Relative volatilities	Ki, distribution coefficient
Lactic acid	5.337	0.476
Water	858.486	76.501
Oligomer/Dilactic acid	9.019	0.804
Lactide	1	0.089

The relative volatilities are expressed respect to the HK component. The information given in table 5 was calculated from data supplied by the engineering program Aspen Plus®.

Table 7. Mass balance results in column T-401. (Own authorship)

STREAM	28	29	30	31
Mass flows (kg/h)				
L-Lactic acid	75.69	6.38	29.10	40.20
D-Lactic acid	8.18	0.69	3.14	4.34
Water	202.07	196.50	5.57	0
L-Lactide	5793.36	118.56	2884.71	2790.09
D-Lactide	625.88	12.81	311.64	301.42
Meso-Lactide	832.12	17.03	414.34	400.75
Oligomer	387.69	104.84	282.85	0
Total mass flows (kg/h)	**7924.98**	**456.81**	**3931.36**	**3536.81**

1.2.5 Column T-402

The mass balance for column T-402 was calculated similarly than the mass balance for column T-401.

Table 8. Mass balance results in column T-402. (Own authorship)

STREAM	30	37	38	39
Mass flows (kg/h)				
L-Lactic acid	29.10	1.07	18.74	9.30
D-Lactic acid	3.14	0.12	2.02	1.00
Water	5.57	5.02	0.55	0
L-Lactide	2884.71	2.79	261.73	2620.19
D-Lactide	311.64	0.30	28.28	283.07
Meso-Lactide	414.34	0.40	37.59	376.35
Oligomer	282.85	24.82	258.03	0
Total mass flows (kg/h)	**3931.36**	**34.52**	**606.94**	**3289.90**

1.2.6 Column T-403

In this column the LK is the meso-lactide and the HK is the inseparable mixture of L-lactide and D-lactide. The LNK (light non key) is the lactic acid. The amount of each enantiomer has been calculated taking into account the racemization.

Table 9. Mass balance results in column T-403. (Own Authorship)

STREAM	47	48	49
Mass flows (kg/h)			
L-Lactic acid	49.50	49.50	0
D-Lactic acid	5.35	5.35	0
Water	0	0	0
L-Lactide	5410.28	44.07	5366.21
D-Lactide	584.49	4.76	579.73
Meso-Lactide	777.10	717.04	60.06
Oligomer	0	0	0
Total mass flows (kg/h)	**6826.71**	**820.71**	**6006.00**

1.2.7 Polymerization reactor R-501

The mass balance in the polymerization reaction has been made for a 0.456 conversion of the monomer, which is 30 min of residence time. The mass balances were calculated in agreement with other the explanations of the Annex II. Supporting Calculations. This reactor and reactor R-502 are operating to carry out the same chemical reaction of polymerization. However, this reactor polymerizes lactide until the conversion indicated and for further conversions reactor R-502 is used.

Table 10. Mass balance results in polymerization reactor R-501. (Own authorship)

STREAM	**51**	**52**	**53**
Mass flows (kg/h)			
L-Lactide	5366.21	0	2903.01
D-Lactide	579.73	0	313.62
Meso-Lactide	60.06	0	32.49
Poly (lactic acid)	0	0	2756.98
Catalyst 2	0	7.85	7.74
Total mass flows (kg/h)	**6006.00**	**7.85**	**6013.85**

1.2.8 Polymerization reactor R-502

Calculations for this reactor are explained in Annex II. Supporting Calculations.

Table 11. Mass balance results in polymerization reactor R-502. (Own authorship)

STREAM	**54**	**55**
Mass flows (kg/h)		
L-Lactide	2903.01	266.45
D-Lactide	313.62	28.79
Meso-Lactide	32.49	2.98
Poly (lactic acid)	2756.98	5707.88
Catalyst 2	7.74	7.74
Total mass flows (kg/h)	**6013.85**	**6013.85**

2. Energy balances

2.1 Introduction to energy balance

An energy balance is a relationship between the energy input, output, consumed and generated in a process, equipment or stage. In regards to the thermodynamics, there are five types of energy: work, heat, internal energy, potential energy and kinetic energy. An energy balance is the result of the application of the first law of thermodynamics, which states that the energy cannot be created or destroyed, but only transformed. The first law of thermodynamics can be expressed as indicated in the equation 10 and shows how the energy is conserved. Similarly to the mass balances, in steady state conditions without generation the energy input is equal to the energy output. [5]

$$\Delta U + \Delta E_p + \Delta E_k = Q - W \tag{10}$$

Where, ΔU = Change in internal energy; ΔE_p = Change in potential energy; ΔE_k = Change in kinetic energy; Q = Heat energy; W = Work.

2.2 Energy balance by equipment

2.2.1 Evaporator E-101

The energy balance in the evaporator can be calculated by considering the general energy equation 10 and taking into account several assumptions: there is no work, the potential energy is negligible despite the inlet and outlet streams are not at the same level and there is no change in kinetics because there is no change in the fluid velocity (assumed).

In the evaporator, the process stream inlet (stream 2) at liquid state partially vaporizes, so the final outlet is more concentrated. This stream is heated with a utility at higher temperature and at different pressure. As the energy is conserved, the utility transfers energy to the process stream. The process stream is heated due to a change in the sensible enthalpy and the latent enthalpy. The heat transfer can be express in agreement with the equations 11 and 12.

$$Q_{boiling} = (F - S)\lambda_E + F\, c_{pf}\, (t_s - t_f) \tag{11}$$

Where,

$Q_{boiling}$ = Heat flow of the boiling chamber (kJ/h).

F = Flow rate of the feed to the evaporator (kg/h).

S =Flow rate of the liquid concentrate (kg/h).

λ_E= Enthalpy of vaporization of the solvent (kJ/kg).

c_{pf} = Heat capacity of the feed solution (kJ/kg ºC).

t_s = Temperature of the liquid concentrate (ºC).

t_f = Temperature of the feed (ºC).

The first term in equation 11 is the latent enthalpy and the second term is the sensible enthalpy.

$$Q_{condensing} = W\, \lambda_w \tag{12}$$

Where,

$Q_{condensing}$ = Heat flow of the condensing chamber (kJ/h).

W = Flow rate water vapor utility (kg/h).

λ_w = Enthalpy of condensation (kJ/kg).

In table 12 is shown the information required for the calculation of the energy balance in the evaporator and in table 13 are collected the final results.

Table 12. Data for the energy calculations in E-101. (Own authorship)

Characteristics of the boiling chamber	
t_f (ºC)	20
t_s (ºC)	95
P (kPa)	6.5
F (kg/h)	12970.71
c_{pf} (kJ/kg ºC)	1.33
λ_E (kJ/kg)	2413.11
Characteristics of the condensing chamber	
P (kPa)	405.3
λ_w (kJ/kg)	2131.5

As $Q_{boiling} = Q_{condensing}$, the flow rate of the low pressure steam can be calculated.

Table 13. Results of the energy calculations in E-101. (Own authorship)

Property	**Value**
$Q_{boiling}$ (kW)	2360.08
$Q_{condensing}$ (kW)	2360.08
W (kg/h)	3520.89

2.2.2 Heat exchanger E-103

The function of this heat exchanger is the heating of the lactic acid aqueous solution to be fed to the pre-polymerization reactor. At 30.5 kPa and at the inlet and outlet temperature of the heat exchanger the stream remains liquid, so there is no phase change. The energetic requirements for this heat exchanger can be calculated in agreement with equation 13.

$$Q = m\,\overline{c_{p,mixture}}\,(t_{out} - t_{in}) \tag{13}$$

Where,

Q = Heat transferred (kJ/h).

m = Flow rate of the process stream (kg/h).

$\overline{c_{p,mixture}}$ = Average specific capacity of the process stream (kJ/kg ºC).

t_{out} = Temperature of the process stream at the outlet (ºC).

t_{in} = Temperature of the process stream at the inlet (ºC).

Table 14. Results and data for the heat exchanger E-103. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	95	T_{in} (ºC)	159.39
T_{out} (ºC)	140	T_{out} (ºC)	159.39
$Cp,_{mixture}$ (kJ/kg ºC)	3.03	P (kPa)	607.95
Flow rate (kg/h)	9986.53	$\lambda_{condensation}$ (kJ/kg)	2083.46
Q (kW)	377.64	Flow rate (kg/h)	652.52

The utility used for this heat exchanger is lps (low pressure stream) at 607.95 kPa and its flow rate can calculated in agreement with equation 12.

2.2.3 Pre-polymerization reactor R-201

The reactor R-201 is a reactor with a continuous flow operation (steady-state). For this case, the general energy equation for a system where the heat is generated can be expressed as shown in equation 14, which is the adaptation of equation 10. [6]

$$F_{A0} \sum_{i=1}^{n} \theta_i \left(H_i - H_{i0}\right) + F_{A0}\, X\, \Delta H_R = Q + W \tag{14}$$

Where,

F_{A0} = Molar flow of the limiting reagent (kmol/h).

θ_i = Relationship F_{i0}/F_{A0}.

H_i = Enthalpy at output conditions (kJ/kmol).

H_{i0} = Enthalpy at input conditions (kJ/kmol).

X = Conversion of the limiting reagent.

ΔH_R = Heat of the reaction (kJ/kmol).

Q = Heat flow (kJ/h).

W = Work flow (kJ/h).

The i index is referred to each of the components involve in the reaction system and for this reactor the heat of reaction is the heat of polymerization, which is expressed per mol of the monomer. Moreover, for a chemical reactor the work done is assumed as W=0.

The enthalpy of polymerization can be estimated with the Hess law applied to the particular reaction equation determined for this reactor.

In order to carry out the energy balances in these reactor with simple calculations equation 3 has been specified for the formation of a 2500 g/mol polymer. A polymer of this molecular weight is formed of 35 lactic acid units (monomer) and two lactic acid monomers acting as end chain, so for its formation approximately 37 molecules of reagent are required for each molecule of polymer formed and 36 molecules of water are released.

The higher the molecular weight of the polymer, the lower the relationship between the molecules of monomer consumed and the water formed. The stoichiometry can be consider 1 to 1 respect to the lactic acid and the water.

In order to estimate de standard enthalpies of formation for the lactic acid and the polymer, the method of Constantinou and Gani was used. This is a group contribution method. The enthalpy of formation is estimated in agreement with equation 15. [7]

$$\Delta H^o{}_f = 10.835 + \left[\sum_k N_k\,(hf1k) + W \sum_j M_j(hf2j) \right] \tag{15}$$

Where,

$\Delta H^o{}_f$ = Standard enthalpy of formation (kJ/mol).

N_k = Number of First- Order groups of type k.

$hf1k$ = Contribution of the First order group 1k for the enthalpy estimation (kJ/mol).

M_j = Number of Second- Order group of type j.

$hf2j$ = Contribution of the Second- Order group 2j for the enthalpy estimation (kJ/mol).

Table 15. First-Order Constantinou /Gani Group Contributions. [7]

Units	CH	CH_3	OH	COOH	COO
Property (kJ/mol)	-3.766	-45.947	-181.422	-396.242	-313.545

Table 16. Data information required for the calculation of the standard enthalpy of reaction.

Material	**$\Delta H_f{}^o$ (kJ/mol)**
Lactic acid	-616.542
Lactic acid monomer unit	-352.423
Poly (lactic acid) monomer end chain	-445.955
Poly (lactic acid) monomer end chain	-544.680
Poly (lactic acid) 2500 g/mol polymer	-13314.605

The enthalpy of polymerization at 180ºC can be calculated in agreement with equation 16.

$$\Delta H_{polymerization} = \Delta H^{o}_{polymerization} + \Delta H_{reactants} + \Delta H_{products} \qquad (16)$$

Where,

$\Delta H^{o}_{polymerization}$ = Standard enthalpy of polymerization at 25ºC and 101.325 kPa.

$\Delta H_{reactants}$ = Enthalpy of the reactants at the input conditions of the reaction system.

$\Delta H_{products}$ = Enthalpy of the products at the input conditions of the reaction system.

Table 17. Data information required for the balance in the reactor R-201. (Own authorship)

Property	Value
Enthalpy of lactic acid at 140ºC (J/kmol)	6.58E+08
Enthalpy of lactic acid at 180ºC (J/kmol)	6.48E+08
Enthalpy of methanol at 140ºC (J/kmol)	1.95E+08
Enthalpy of methanol at 180ºC (J/kmol)	1.93E+08
Enthalpy of water at 140ºC (J/kmol)	-2.38E+08
Enthalpy of water at 180ºC (J/kmol)	-2.37E+08
Standard enthalpy of polymerization (kJ)	-1693.69
Standard enthalpy of polymerization (kJ/mol)	-45.78
Enthalpy of the products due to heating (kJ)	7.72
Enthalpy of the reactants due to cooling (kJ)	-30.86
Enthalpy of polymerization (kJ)	-1716.88
Enthalpy of polymerization (kJ/mol)	-46.40

Table 18. Final results of the energy balance in the reactor R-201. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
Q (kW)	-74176.90		
T_{in} (ºC)	140.00	T_{in} (ºC)	32.22
T_{out} (ºC)	180.00	T_{out} (ºC)	152.34
Cp_{Water} (kJ/kg ºC)	4.63	P (kPa)	506.63
λ_{water} (kJ/kg)	2106.54	Flow rate (kg/h)	100303.60

This reactor is refrigerated with an evaporative cooling: water enters the reactor for refrigeration and low pressure steam leaves the reactor.

2.2.4 Stirrer storage tank V-301

The stirrer storage tank V-301 is the equipment where the stream 16 is mixed with the respective streams containing the catalyst and the stabilizer, so as with stream 17 coming from the depolymerisation reactor, which is a recycle stream. This tank has to be maintained at 160ºC, so the equipment requires a cooling jacket for refrigeration. The balance on this equipment can be made taking into account the following assumptions:

- The energy balance in the stirrer storage tank is an energy balance for an open system with multiple inputs and one output.
- The catalyst and stabilizer stream are considered negligible for the balance.
- There is no enthalpy change due to mixing.
- The non-volatile materials are not considered for the calculation of the heat capacities of the streams.

The energy balance in the stirrer storage tank can be expressed as indicated in equation 17. [6]

$$Q = \sum_{i=1}^{n} m_i h_i - \sum_{j=1}^{n} m_j h_j \tag{17}$$

Where,

m_i = Flow rate of the input i (kg/h).

H_i = Enthalpy of the input i (kJ/kg).

m_j = Flow rate of the output j (kg/h).

h_j = Enthalpy of the output j (kJ/kg).

The change of the enthalpies can also be expressed as a heat capacity by a difference of temperature. The enthalpies are related, then, to a change of the sensible heat.

Table 19. Information for the energy balance in V-301. (Own authorship)

STREAM **Property**	**16**	**17**	**20**
T (ºC)	180	220	160
m_i (kg/h)	8090.57	3169.12	11260.89
Cp_i (kJ/kg ºC)	285.24	61.84	220.78

Table 20. Results for the energy balance in V-301. (Own authorship)

UTILITY	
Property	**Value**
Q (kW)	-21.66
T_{in} (ºC)	32.22
T_{out} (ºC)	48.89
P (kPa)	101.33
Flow rate (kg/h)	14122.70

The refrigeration utility is cooling water.

2.2.5 Heat exchanger E-301

This heat exchanger heats the low molecular weight poly (lactic acid) with the catalyst and the stabilizer (streams 21 and 22) to be fed to the depolymerization reactor. The operating pressure is 35 kPa. The utility used for this heat exchanger is saturated vapour at 4136.85 kPa and 252.33 ºC. The calculations can be made in agreement with equations 12 and 13.

Table 21. Results and data for the heat exchanger E-302. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	160	T_{in} (ºC)	252.33
T_{out} (ºC)	220	T_{out} (ºC)	252.33
$Cp_{,mixture}$ (kJ/kg ºC)	0.37	$\lambda_{condensation}$ (kJ/kg)	1701.38
Flow rate (kg/h)	11260.89	P (kPa)	4136.85
Q (kW)	70.22	Flow rate (kg/h)	148.59

2.2.6 Depolymerization reactor R-301

The depolymerization reactor R-301 is an isothermic reactor which operates at 220ºC and at 2.5 kPa. The energy balance in this reactor has a similar procedure to the energy balance previously explained for reactor R-201. Equation 14 must be considered again, however, in this case, the enthalpy change of the reagents being introduced and leaving the reactor are insignificant. For this reason, all the energy supply to the reactor can be calculated only taking into account the heat of the reaction.

The heat of the reaction must be calculated for the main reaction (PLA to form lactide) and the considered side reactions (lactic acid to form dilactic acid). One lactide is formed from two lactic acid units. Accordingly, one polymer chain of poly (lactic acid) of 2500 g/mol forms 18.5 molecules of lactide.

The standard enthalpy of formation for lactide is -672.59 kJ/mol and for dilactic acid is -993.93 kJ/mol.

Table 22. Data information require for the balance in reactor R-301. (Own authorship)

Property	Value
Standard enthalpy of the main reaction (kJ)	871.69
Standard enthalpy of the main reaction (kJ/mol PLA)	871.69
Enthalpy of the products due to heating of the main reaction (kJ)	46.11
Enthalpy of the reactants due to cooling of the main reaction (kJ)	-9.69
Enthalpy of the main reaction (kJ)	908.28
Enthalpy of the main reaction (kJ/mol PLA)	908.28
Standard enthalpy of the side reaction (kJ)	-46.65
Standard enthalpy of the side reaction (kJ/mol LA)	-23.33
Enthalpy of the side reaction (kJ)	-10.23
Enthalpy of the side reaction (kJ/mol LA)	-5.11

Table 23. Final results of the energy balance in the reactor R-301. (Own authorship)

UTILITY	
Property	**Value**
Q (kW)	155.11
$\lambda_{condensation}$ (kJ/kg)	1701.38
T_{in} (ºC)	252.33
T_{out} (ºC)	252.33
P (kPa)	4136.85
Flow rate (kg/h)	328.20

2.2.7 Heat exchanger E-302

The vapour outlet stream of the reactor R-301 (stream 27) must be cooled with the heat exchanger E-302. The utility used is cooling water at 32.22ºC and atmospheric pressure. The temperature must be reduced from 232.07 ºC to 120 ºC (temperature of the feed of the column T-401). At the operating pressure of the heat exchanger (6 kPa) the boiling temperature of the water, lactic acid, lactide and dilactic acid is 36.15 ºC, 145.46 ºC, 177.2 ºC, 138.67 ºC respectively. For this reason, the heat exchanger cannot condense the water and the feeding to column T-301 is almost liquid with a 13% of vapour.

Table 24. Data for the calculation in the heat exchanger E-302. (Own authorship).

	Property	Value
Vapour	Cp_{water}(kJ/kg ºC)	1.92
	$Cp_{dilactic\ acid}$ (kJ/kg ºC)	1.46
	$Cp_{lactic\ acid}$ (kJ/kg ºC)	1.54
	$Cp_{lactide}$(kJ/kg ºC)	1.52
Liquid	$Cp_{lactide}$ (kJ/kg ºC)	3.98
	$Cp_{dilactic\ acid}$ (kJ/kg ºC)	3.89
	$Cp_{lactic\ acid}$ (kJ/kg ºC)	5.92
	$\lambda_{lactic\ acid}$ (kJ/kg)	7.93
	$\lambda_{dilactic\ acid}$ (kJ/kg)	393.45
	$\lambda_{lactide}$ ((kJ/kg)	517.39

Table 25. Results for the heat exchanger E-302 (Own authorship).

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	232.07	T_{in} (ºC)	32.22
T_{out} (ºC)	120	T_{out} (ºC)	48.89
Flow rate (kg/h)	7924.98	$Cp_{,water}$ (kJ/kg ºC)	4.18
Q (kW)	1770.38	Flow rate (kg/h)	91385.54

2.2.8 Column T-401

The energy balance in a distillation column can be calculated taking into account that all the energy input is equal to the energy output because there is no generation of energy, and in agreement with the first law of thermodynamics, the energy is conserved. The energy balance can be calculated with equations 19 and 20.

$$Q_R + F\,h_F = D_{vapour}H_D + D_{liquid}h_D + B\,h_B + Q_C + Q_{column} \tag{18}$$

Where,

Q_R = Heat transfer in the reboiler (kJ/h).

F = Flow rate of the feed of the column (kmol/h).

h_F = Enthalpy of the feed of the column (kJ/kmol).

D_{vapour} = Flow rate of the vapour distillate (kmol/h).

H_D = Enthalpy of the vapour distillate (kJ/kmol).

D_{liquid} = Flow rate of the liquid distillate (kmol/h).

h_D = Enthalpy of the liquid distillate (kJ/kmol).

B = Flow rate of the bottoms stream (kmol/h).

h_B = Enthalpy of the bottoms stream (kJ/kmol).

Q_C = Heat transfer in the condenser (kJ/h).

Q_{column} = Heat transfer due to losses in the column (kJ/h).

$$V_1 H_1 = D_{vapour} H_D + D_{liquid} h_D + L_0\, h_0 + \; Q_c \tag{19}$$

Where,

V_1 = Flow rate of the vapour stream in the top of the column (kmol/h).

H_1 = Enthalpy of the vapour stream in the top of the column (kJ/kmol).

L_0 = Reflux flow rate liquid (kmol/h).

h_0 = Enthalpy of the reflux liquid stream (kJ/kmol).

The heat transfer due to the losses of energy in the column can be considered negligible. The column is assumed to be well isolated. If all enthalpies and flow rates of the input and output streams are known, the energies exchange in the reboiler and the condenser are calculated.

Table 26. Information required for the energy balance in the column T-401. (Own authorship)

STREAMS	**PROPERTIES**		
	Molar flow rate (kmol/h)	**Temperature (ºC)**	**Enthalpy (kJ/kmol)**
F	64.85	120	670775
$D_{,liquid}$	27.46	112	764400
$D_{,vapour}$	12.66	112	315229
B	24.72	152	737113
V_1	56.60	144	645484
L_0	16.48	112	764400

All the enthalpies shown in table 26 has been estimated with Aspen Plus®.

Table 27. Final results for column T-401. (Own authorship)

Condenser E-401		**Reboiler E-402**	
Q_C (kW)	-289.92	Q_R (kW)	370.60
T_{in} (ºC)	32.22	T_{in} (ºC)	165.67
T_{out} (ºC)	48.89	T_{out} (ºC)	165.67
Flow rate (kg/h)	14965.21	Flow rate (kg/h)	1078.47

The condenser uses cooling water as refrigeration media and the reboiler uses medium pressure steam at 709.28 kPa.

2.2.9 Column T-402

The energy balance in column T-402 can be solved also in accordance to equations 19 and 20. The balances were calculated with the same procedure explained for column T-401.

Table 28. Information for the energy balance in the column T-402. (Own authorship)

STREAMS	**PROPERTIES**		
	Molar flow rate (kmol/h)	**Temperature (°C)**	**Enthalpy (kJ/kmol)**
F	27.46	112	764400
$D_{,liquid}$	4.13	112	866176
$D_{,vapour}$	0.47	112	518590
B	22.87	153.6	737894
V_1	29.35	144	795089
L_0	24.75	112	866176

Table 29. Final results for column T-402. (Own authorship)

Condenser E-404		**Reboiler E-405**	
Q_C (kW)	-534.18	Q_R (kW)	617.97
T_{in} (ºC)	32.22	T_{in} (ºC)	165.67
T_{out} (ºC)	48.89	T_{out} (ºC)	165.67
Flow rate (kg/h)	27574.16	Flow rate (kg/h)	1078.47

The condenser uses cooling water as refrigeration media and the reboiler uses medium pressure steam at 709.28 kPa.

2.2.10 Heat exchanger E-407

This heat exchanger reduces the temperature from 152.77 ºC to 120 ºC. It is an equipment required for the conditioning of the feeding to the column T-403. The stream 46 is introduced in the heat exchanger E-407 as liquid and remains as liquid because there is no phase change. The utility needed for refrigeration is cooling water.

Table 30. Calculation results and data for the heat exchanger E-407. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	152.77	T_{in} (ºC)	32.22
T_{out} (ºC)	120.00	T_{out} (ºC)	48.89
$Cp,_{mixture}$ (kJ/kg ºC)	1356.00	Cp_{water} (kJ/kg ºC)	4.18
Flow rate (kg/h)	6826.71	Flow rate (kg/h)	4349.89
Q (kW)	84.27		

2.2.11 Column T-403

Column T-403 can also be solved with equations 19 and 20, however there is only a liquid distillate in this column because the column operates with a total condenser. Therefore, equations 19 and 20 were adjusted for this particular case.

Table 31. Information for the energy balance in the column T-403. (Own authorship)

STREAMS	**PROPERTIES**		
	Molar flow rate (kmol/h)	**Temperature (ºC)**	**Enthalpy (kJ/kmol)**
F	47.59	120	747036
D	5.92	132.97	735684
B	41.67	141.82	741800
V_1	9.48	132.97	643790
L_0	3.55	132.97	735684

The L-lactide, D-lactide and meso-lactide enthalpy for the estimation of the enthalpy of the streams of the column T-403 with Aspen Plus® has been considered similar in the three cases.

Table 32. Final results for column T-403. (Own authorship)

Condenser E-408		**Reboiler E-409**	
Q_C (kW)	-241.89	Q_R (kW)	162.61
T_{in} (ºC)	32.22	T_{in} (ºC)	165.67
T_{out} (ºC)	48.89	T_{out} (ºC)	165.67
Flow rate (kg/h)	12486.30	Flow rate (kg/h)	283.78

The condenser uses cooling water as refrigeration media and the reboiler uses medium pressure steam at 709.28 kPa.

2.2.12 Heat exchanger E-410

Heat exchanger E-410 increases the temperature from 141.82 ºC to 180ºC which is temperature of the operation of the reactor R-501. The pressure of operation of this equipment is 30 kPa, pressure at which the boiling temperature of the lactide is 217.66 ºC. Accordingly, the stream 51 is completely liquid. The heating media is high pressure steam.

Table 33. Results and data for the heat exchanger E-410. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	141.82	T_{in} (ºC)	229.21
T_{out} (ºC)	180	T_{out} (ºC)	229.21
$Cp_{lactide}$ (kJ/kg ºC)	2.00	P (kPa)	2757.90
Flow rate (kg/h)	6006.00	$\lambda_{condensation}$ (kJ/kg)	1815.28
Q (kW)	127.30	Flow rate (kg/h)	252.46

2.2.13 Polymerization reactor R-501

The energy balance in Reactor R-501 has been calculated with a similar procedure of reactor R-301. Both are isothermic reactors where the enthalpy change is completely negligible. In other words, the equation 14 becomes the equation 20.

$$F_{A0}\, X\, \Delta H_R = Q \tag{20}$$

The enthalpy of reaction or enthalpy of polymerization is -22.9 kJ/mol and the conversion for this reactor is 0.459. The final results are introduced in table 34.

Table 34. Results and data for the reactor R-501. (Own authorship)

Property	**Value**
Q (kW)	-121.68
T_{in} (ºC)	32.22
T_{out} (ºC)	48.89
Cp (kJ/kg ºC)	4.18
P (kPa)	1013.25
Flow rate (kg/h)	6280.86

The results of table 34 provides the information of the heat to be removed and the specifications of the utility required (cooling water).

2.2.14 Polymerization reactor R-502

The equation 20 can also be used for the calculation of the energy balance of this reactor. However, the reagent (lactide) is partially converted to polylactic acid in this case. For this reason, the equation 20 is slightly transformed.

$$F_{A0}\ (X_{out} - X_{in})\ \Delta H_R = Q \tag{21}$$

Table 35. Results and data for the reactor R-501. (Own authorship)

Property	**Value**
Q (kW)	-130.24
T_{in} (ºC)	32.22
T_{out} (ºC)	48.89
Cp (kJ/kg ºC)	4.18
P (kPa)	1013.25
Flow rate (kg/h)	6722.91

2.2.15 Heat exchanger E-601

Heat exchanger E-601 increases the temperature from 180 ºC to 220 ºC which is the temperature required for volatilization. The pressure of operation of this equipment is 30 kPa. The lactide is in vapour phase at the output temperature. A change of phase is expected for lactide and other compounds like 1-dodecanol and phosphoric acid.

Table 36. Results and data for the heat exchanger E-601. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	180.00	T_{in} (ºC)	240
T_{out} (ºC)	220	T_{out} (ºC)	240
$Cp,_{mixture}$ (kJ/mol ºC)	0.15	P (kPa)	3347.80
Flow rate (kg/h)	6014.35	$\lambda_{condensation}$ (kJ/kg)	1763.50
Q (kW)	10059.52	Flow rate (kg/h)	20535.45

The utility used in this heat exchanger is high pressure steam. More information is provided in table 36.

2.2.16 Heat exchanger E-102

This heat exchanger condenses part of the vapor of the stream 5. It is located between two ejectors and its main function, with the vapor-liquid phase separator V-101, is to reduce the load of flow rate introduced to the second ejector.

Table 37. Properties at 50 kPa for the energy balance in E-102. (Own authorship)

	Boiling point (ºC)	Heat capacity for liquid (kJ/kg ºC)	Heat capacity for vapor (kJ/kg ºC)	Enthalpy of vaporization (kJ/kg)
Lactic acid	195.85	3.027	1.461	880.34
Methanol	47.61	5.859	1.665	1044.75
Water	81.34	5.247	1.914	2285.05

Table 38. Results and data for the heat exchanger E-102. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	209.49	T_{in} (ºC)	32.22
T_{out} (ºC)	85.00	T_{out} (ºC)	48.89
Flow rate (kg/h)	2984.18	Cp (kJ/kg ºC)	4.18
Q (kW)	343.08	Flow rate (kg/h)	17709.44

2.2.17 Heat exchanger E-403

Heat exchanger E-403 has the same function of the heat exchanger E-102. The stream 29 is partially liquefied at 15 kPa. Calculations for this heat exchanger and heat exchanger E-406 are analogous.

Table 39. Properties at 15 kPa for the energy balance in E-403 and E-406. (Own authorship)

	Boiling point (ºC)	Heat capacity for liquid (kJ/kg ºC)	Heat capacity for vapour (kJ/kg ºC)	Enthalpy of vaporization (kJ/kg)
Lactic acid	165.35	2.976	1.490	763.32
Lactide	199.15	2.095	1.418	501.78
Dilactic acid	160.18	2.005	1.409	381.49
Water	53.97	5.306	1.918	2081.69

Table 40. Results and data for the heat exchanger E-403. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	204.49	T_{in} (ºC)	32.22
T_{out} (ºC)	112.00	T_{out} (ºC)	48.89
Flow rate (kg/h)	456.81	Cp (kJ/kg ºC)	4.18
Q (kW)	48.93	Flow rate (kg/h)	2525.84

2.2.18 Heat exchanger E-406

The energy balance is calculated with the same procedure that heat exchanger E-403.

Table 41. Results and data for the heat exchanger E-410. (Own authorship)

PROCESS STREAM		UTILITY	
Property	**Value**	**Property**	**Value**
T_{in} (ºC)	197.94	T_{in} (ºC)	32.22
T_{out} (ºC)	112.00	T_{out} (ºC)	48.89
Flow rate (kg/h)	34.52	Cp (kJ/kg ºC)	4.18
Q (kW)	3.89	Flow rate (kg/h)	200.79

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ANNEX II

Supporting calculations

Index

1. Introduction

The equipment chosen for design in this project is the reactor R-502, which is the unit to be detailed in the next sections of the Annex II: Supporting calculations.

A reactor is the equipment in where some initial raw materials called reactants are transformed by energy supply or energy removal in other materials called products. Accordingly, a reactor is the vessel or container in where the reactive system of a process is developed in agreement with some chemical reactions.

The design of this equipment must be performed taking in mind some basic objectives. The type of reactor must be selected regarding the process type and the operating mode. The reactive system conditions must be known. In this way the pressure, temperature and the compositions during the operation of a reactor must be known.

From this basic objectives, the design must focus on the reactor sizing and the definition of its structural compounds (mechanical design), the compositions and the physical conditions of the product (material balances), the heat transfer determination (energy balances), the kinetics determination and the elements modifying those kinetics (catalysts).

In order to carry out a good design all chemical engineering basic principles are assess: mass transfer, heat transfer, fluids flow, mechanical design, economy and safety in design and in operation.

This annex also includes a basic sizing of the rest of the equipment of this project. The thermal or mechanical design, as required, is not specified for other equipment than reactor R-502.

2. Polymerization reactor R-502

2.1 Selection of the reactor type

Nowadays, there are different types of reactor configurations. The most common are the tubular reactors, the stirred tank reactors, the fixed bed catalytic reactors, the fixed-bed non catalytic reactors, the moving bed catalytic reactors, the fluidized bed catalytic reactors, the fluidized bed non catalytic reactors and the kilns.

As, the catalyser required for the reaction is found in solution with the process materials to introduce in the reactor, the possible reactor configurations to be examined are the tubular and stirred tank reactors.

High viscosity and heat transfer are the main aspects to take into account for the reactor selection. Chemical industries can handle viscosities within a range of 50,000 to 10 million Cp. Reactor R-502 is processing a fluid with an expected maximum viscosity of approximately 1,6 million Cp, which is a very high viscosity.

Heat transfer in viscosity fluids may become a challenge because, as the viscosity increases, the heat transfer coefficients sharply decreases. Polymerization reactions, such as the one expected for PLA production, are exothermic and require and a good heat transfer in order to avoid the polymer degradation and possible runaways. The heat transfer in stirred tank reactors initially increases with the agitation speed of the impeller however, as the viscosity increases and the impeller speed increases (the agitation supplies a certain amount of heat to the process), the heat removed decreases.

The chosen reactor must be then a plug flow reactor or tubular reactor. The high heat transfer surface area per volume allows for high rates of heat transfer and the reactor stays isothermal. Moreover, they can control the residence time very carefully, which is an important aspect for the final molecular weight of the polymer. The configuration for the reactor is then, multitubular.

2.2 Chemistry of the reactor R-502

2.2.1 Kinetics equations for polymerization

The continuation of the polymerization previously started in reactor R-501 is happening inside reactor R-502. This polymerization allows the conversion of lactide into a high molecular weight poly (lactic acid). Therefore, the reactant monomer of the polymerization is a cyclic ring which is being transformed by a ring-opening mechanism into a polymer.

The cyclic monomer must react first with an initiation agent in order to start the polymerization. New active species are produced with the ring opening of lactide which will progressively build a polymer chain with the addition of new monomers. This phenomena is called propagation reaction. Side reactions can occur during the polymerization like termination or deactivation of the polymer, transesterification and pyrolytic elimination. Five types of reaction can be identified during polymerization in this reactor:

1. Reversible activation reaction.
2. Reversible propagation reaction.
3. Reversible termination reaction.
4. Transesterification reaction.

5. Non-radical random chain scission reactions.

The activation reaction allows for the production of activated species that ensure the polymerization starting. The cyclic monomer activation is performed with a catalyst and an R-OH co-catalyst type which, as a whole, form the initiator agent group. This agent is completely activated when the co-catalyst is in excess.

$$C + S \xleftrightarrow{k_{a1}, k_{a2}} I + A \tag{1}$$

$$C + P_j \xleftrightarrow{k_{a1}, k_{a2}} R_i + A \tag{2}$$

Where, C = catalyst; S = Solvent concentration, co-catalyst; I = initiator; A = acid; R_i = Active polymer chain; P_j = Dormant polymer chain.

The reversible propagation reaction is the main reaction of this reactive system of polymerization. The polymer can grow taking into account this reaction type. Equation 3 is considered to be the initiation reaction.

$$I + M \xleftrightarrow{k_p, k_d} R_1 \tag{3}$$

$$R_i + M \xleftrightarrow{k_p, k_d} R_{i+1} \tag{4}$$

Where M = Cyclic monomer of lactide; R_1 = Initial active specie; k_p = Propagation constant; k_d = Depropagation constant.

There are also reversible chain transfer reactions. The activated species, both monomeric and polymeric, reacts with the R-OH species added as a co-catalyst during this reactions. An inactive polymeric chain and a new active specie are, then, formed. In the latter case, the active specie will react again and the propagation reaction can start over. The final concentration of inactive and activated chains will be equal to the initial concentration of the co-catalyst.

$$R_i + S \xleftrightarrow{k_{ts1}, k_{ts2}} R_1 + P_j \tag{5}$$

Where, k_{ts1} = Direct chain transfer to solvent constant; k_{ts2} = Reverse chain transfer to solvent constant.

The reactions indicated in equations 6, 7 and 8 are transesterification reactions. All of them are side reactions with a strong effect on the molecular weight of the polymer, although the chain number remains stable.

$$R_i + R_j \overset{k_{te}}{\leftrightarrow} R_{i+j-k} + R_k \tag{6}$$

Where, R_i,R_j,R_{i+j-k},R_k = Active polymer chains of different molecular weight; k_{te}= Direct and reverse reaction constant.

$$R_i + P_j \overset{k_{te}}{\leftrightarrow} R_{i+j-k} + P_k \tag{7}$$

$$R_i + G_j \overset{k_{te}}{\leftrightarrow} R_{i+j-k} + G_k \tag{8}$$

Where P_j and P_k = Dormant polymer chain of different molecular weights; G_j and G_k = Terminate polymer chain.

Finally, this reactive system also includes the irreversible non-radical random chain scissions. Latent, activated and end chains are degraded by means of these reactions to produced shorter chains of polymer. However, if a living behaviour is assumed for this specific polymerization, the equations 2, 4 and 6 are consider to be the most important and the rest of reactions are completely negligible. [1]

$$R_i \overset{k_{de}}{\longrightarrow} R_{i-k} + G_k \tag{9}$$

$$P_i \overset{k_{de}}{\longrightarrow} P_{i-k} + G_k \tag{10}$$

$$G_k \overset{k_{de}}{\longrightarrow} G_{k-j} + G_j \tag{11}$$

The analysis of the reaction system required for the operation of the reaction R-502 has been shown before. However, for further analysis the living behaviour of the polymerization is assumed. In other words, the number of growing chains remains constant during the polymerization. Moreover, other hypothesis are also consider: the density of the reaction remains constant, the reaction rate constants are independent of the chain length, each initiator agent initiates a polymer chain and the termination of the polymerization is happening by transference with the monomer and the solvent and is also irreversible and dependant of the reactants concentrations. [2]

2.2.2 Kinetic constant of reactions

The reaction rate and equilibrium constants of the main reactions of the defined polymerization system are obtained from experimental data at different temperatures. Therefore, some data has been taken from bibliography. [3]

Table 1. Propagation reaction rate and equilibrium constants for different temperatures. [3]

Temperature (ºC)	k_p (L/ mol h)	$K_{eq,a}$
130	4500	0.045
145	10000	0.101
160	17500	0.126
180	37000	0.256

The reaction rate constant dependency with the temperature is expressed by a mathematical equation named as Arrhenius equation.

$$k = k_0 \, e^{\left(\frac{-E_a}{R\,T}\right)} \tag{12}$$

Where,

k = kinetic constant.

k_0 = Pre-exponential factor or frequency factor.

E_a = Activation energy (J/mol).

R = Universal constant of gases (J/ mol K).

T = Absolute temperature (K).

The activation energy and the pre-exponential factor for the data shown in table 1 can be estimated with a plot where the natural (Naperian) logarithm of the reaction constant rate is plotted in a graphic representation with the inverse of the absolute temperature (for example, ln(k_p) versus the 1/T).

The depropagation rate constant can be calculated in agreement with equation 13.

$$[M]_{eq} = \frac{k_d}{k_p} \tag{13}$$

Where,

$[M]_{eq}$ = Concentration of the monomer in the equilibrium (mol/L).

k_p = Propagation rate constant (L/mol h).

k_d = Depropagation rate constant (h^{-1}).

The depropagation rate constant acquires significance for monomer rings of high size like lactide, which is a 6 member monomer ring. [4]

Polymerization reactions are reversible reactions which are thermodynamically possible when the Gibbs energy is negative and when $\Delta G_p = 0$, which indicates the equilibrium of the reaction. The concentration of the monomer in the equilibrium can be calculated from this assumption.

$$[M]_{eq} = \exp\left(\frac{\Delta H_p^o}{R\,T} - \frac{\Delta S_p^o}{R}\right) \tag{14}$$

Where,

ΔH_p^o = Standard enthalpy of polymerization (J/mol).

ΔS_p^o = Standard entropy of polymerization (J/mol K).

All the model kinetic parameters explained above and other are collected in table 2.

Table 2. Model kinetic parameters. [5]

Rate parameters	**Value at 180ºC**
$k_p = 2.06 \cdot 10^8\ [L\,mol^{-1}s^{-1}] \exp\left(-\frac{63247.09\ [J\,mol^{-1}]}{RT}\right)$	10.28 $[L\,mol^{-1}s^{-1}]$
$k_d = 6.61 \cdot 10^7\ [s^{-1}] \exp\left(-\frac{63247.09\ [J\,mol^{-1}]}{RT}\right)$	3.38 $[s^{-1}]$
$K_{eq,a} = 1.54 \cdot 10^5 \exp\left(-\frac{50127.60\ [J\,mol^{-1}]}{RT}\right)$	0.256
$k_{a1} = 1000\ k_p$	10280 $[L\,mol^{-1}s^{-1}]$
$k_{a2} = \frac{k_{a1}}{K_{eq}}$	40156.25 $[L\,mol^{-1}s^{-1}]$
$k_{te} = 9.39 \cdot 10^7\ [L\,mol^{-1}s^{-1}] \exp\left(-\frac{63247.09\ [J\,mol^{-1}]}{RT}\right)$	4.81 $[L\,mol^{-1}s^{-1}]$
$k_{s1} = k_{s2} = 1000\ k_p$	10280 $[L\,mol^{-1}s^{-1}]$

2.2.3 Molar mass distribution of the polymer during the equilibrium

The molar mass distribution of a polymer is described with a distribution function. Large ring monomers like lactide forms a high molecular weight polymer best described by the Flory-Schultz distribution function. [4]

$$DI = \frac{M_w}{M_n} = \frac{DP_w}{DP_n} = 2 - \frac{1}{DP_n} = 2 - \frac{1}{M_n M_M} \tag{15}$$

Where,

DI = Dispersity index.

M_w = Weight-average molecular weight of the polymer (g/mol).

M_n = Number-average molecular weight of the polymer (g/mol).

DP_w = Weight-average degree of polymerization.

DP_n = Number-average degree of polymerization.

M_M = Molecular weight of the monomer repeating unit (mol/l).

The lactide polymerization has, as assumed, a living behaviour despite the high equilibrium concentration of the monomer. The dispersity index is very close to a value of 2 because of the high molecular weight achieved by the polymer, the high conversions of the monomer and kinetically controlled conditions for polymerization.

2.2.4 Rate for polymerization

The number-average molecular weight of the growing polymer can be expressed as function of the monomer conversion when the rate constant of initiation of the polymerization is expected to be larger than the rate constant of propagation.

$$M_n = \frac{[M]_0 - [M]}{[M]_0} \frac{[M]_0}{[R^*] + [S]} M_M \tag{16}$$

Where,

$[M]_0$ = Initial concentration of the monomer (mol/l).

$[M]$ = Final concentration of the monomer (mol/l).

$[R^*]$ = Concentration of active chains (mol/l).

$[S]$ = Concentration of the co-catalyst or dormant chains (mol/l).

The rate of polymerization can be expressed as indicated in equation 17 when the previous assumptions are taken. Then, the propagation and depropagation reactions are the most important reactions in the polymerization process, as indicated in equation 4.

$$R_p = -\frac{d\,[M]}{dt} = k_p \sum_{i=0}^{\infty} [R_i]\ [M] - k_d \sum_{i=0}^{\infty} [R_i] \tag{17}$$

The integration of equation 17 gives as final result the equation 18.

$$\ln\frac{[M]_0-[M]_{eq}}{[M]-[M]_{eq}} = k_p\sum_{i=0}^{\infty}[R_i]\ \mathrm{t} = k_p\,[R^*]\,t \tag{18}$$

Where,

t = time of polymerization (s).

As a living polymerization is considered, the concentration of living/growing chains remains constant with respect to the concentration of the initial species.

Accordingly,

$$[R^*] = \sum_{i=0}^{\infty}[R_i] \tag{19}$$

$$[S] = \sum_{i=0}^{\infty}[P_i] \tag{20}$$

The final concentration of the co-catalyst is equal to the final concentration of the dormant chains and the concentration of living species is equal to the final concentration of active chains.

A mass balance can be applied for the active chains, the catalyst, dormant chains (concentration of co-catalyst as indicated in equation 20) and acid for equation 2. As a result, the expression of equation 21 is obtained. [3]

$$[R^*] = [S]_0-[S] = [C]_0-[C] = [A]-[A]_0 \tag{21}$$

Where,

[A] =Final concentration of the octanoic acid (mol/l).

$[A]_0$ = Initial concentration of the octanoic acid (mol/l).

$[C]$ = Final concentration of the catalyst (mol/l).

$[C]_0$ = Initial concentration of the catalyst (mol/l).

$[S]_0$ = Initial concentration of the co-catalyst (mol/l).

The final concentration and conversion of the monomer in the polymerization reaction is calculated from equation 18 for a fixed temperature and amount of catalyst and co-catalyst. The molecular weight can be estimated from equations 15 and 16.

The change in the polymerization reaction rate, the propagation and deprogration rate are shown in figure 1. The depropagation rate becomes higher than the propagation rate for a conversion of 0.95 at approximately 200ºC. If operations at 200ºC where required a lower conversion must be chosen due to thermodynamic constraints.

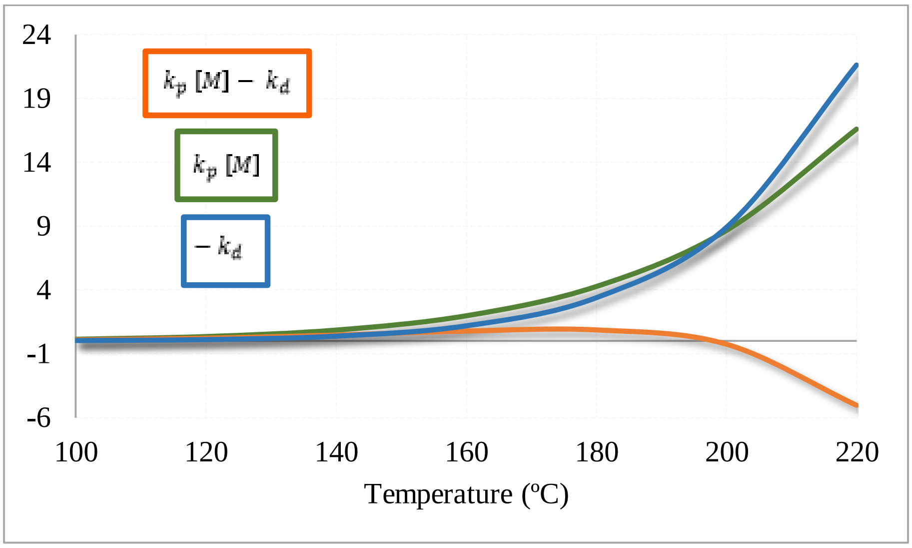


Figure 1. Change of reaction rate $R_p/[R^*]$ (h^{-1}) at 0.95 conversion. (Own authorship)

2.2.5 Conversion, viscosity and time of polymerization

The conversion of the monomer has a strong relationship with the polymerization time, the viscosity of the polymer and the molecular weight of the polymer. These relationships are shown in figures 2 and 3.

The viscosity of the polymer can be estimated from an experimental equation taken from the bibliography. [6] The assumption of zero shear viscosity has been considered for these calculation and the equation is suitable for poly (lactic acid) at 180ºC. The units of the viscosity for equation 22 are Pa·s.

$$\log \eta = -14.26 + 3.4\log(M_w) \tag{22}$$

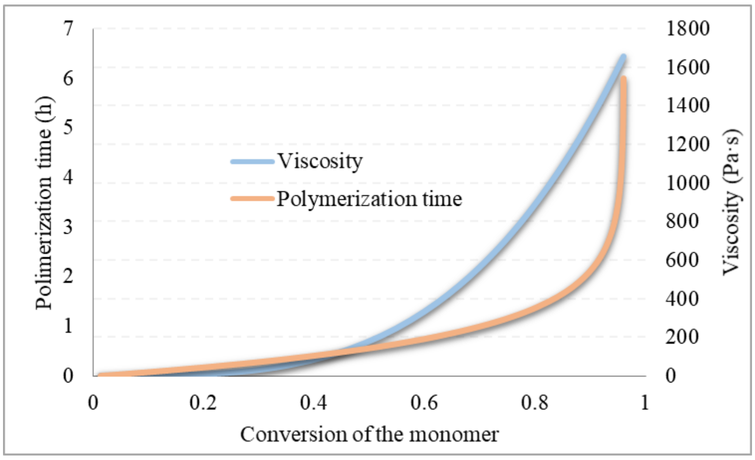


Figure 2. Relationship between the monomer conversion and the polymerization time and viscosity. (Own authorship)

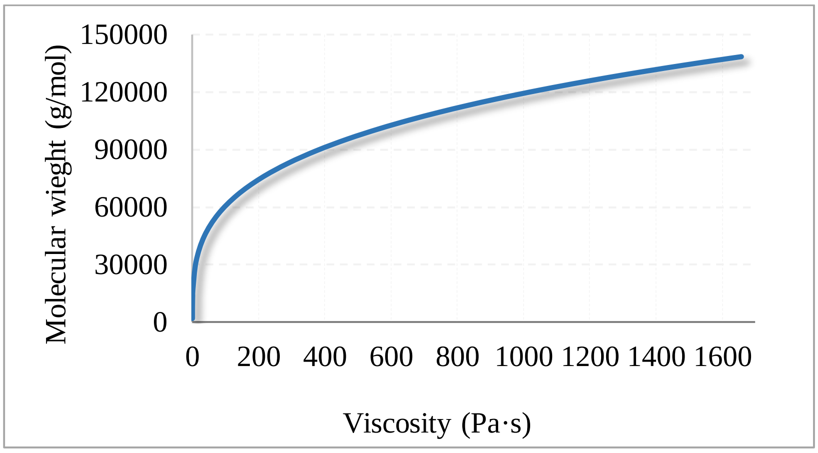


Figure 3. Relationship between the molecular weight and viscosity. (Own authorship)

2.3 Characteristics of the catalyst

2.3.1 Introduction to the catalyst and specifications

Nowadays, there are different types of catalyst able to cause the ring opening of the lactide in order to produce poly (lactic acid) polymer. The chosen catalyst for this chain growth polymerization is $Sn(Oct)_2$, also named as 2-ethylhexanoic acid tin(II). This is a very good catalyst for this process due to its low toxicity, its high solubility in lactide (so a bulked polymerization is allowed), high catalytic selectivity, high monomer conversion and low racemization. The $Sn(Oct)_2$ catalyst has the structure shown in figure 4.

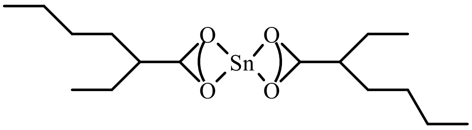


Figure 4. Structure of the tin octoate catalyst $Sn(Oct)_2$. [3]

The catalyst used for reactors R-501 and R-502 has the following specifications explained in table 3.

Table 3. Reaxis® C129 Stannous Octoate catalyst specifications. [7]

Physical State	Liquid
Chemical State	Inorganic tin
Tin (II) content (%)	27.2-29.3
Tin (II)/ Total tin content (%)	97.0 Minimum
Colour (Gardner number)	3 Maximum
Density (g/ml)	1.23-1.27
Viscosity (cp at 25ºC)	400 Maximum
Molecular weight (g/mol)	405.12 g/mol

Despite the numerous advantages, the catalyst must go hand in hand with a co-catalyst for its activation. The co-catalyst is an alcohol because the catalytic agent required for the polymerization reaction is not $Sn(Oct)_2$, but Sn (II) alcoxide, which is formed from the catalyst and the co-catalyst (1-dodecanol for this reaction). The catalyst activation is carried out as summarized in equation 1 and indicated in equations 23, 24 and 25. [4]

$$Sn(Oct)_2 \ + ROH \ \leftrightarrow OctSnOR + OctH \tag{23}$$

$$OctSnOR + ROH \ \leftrightarrow Sn(OR)_2 + OctH \tag{24}$$

$$\ldots - Sn - OR + M \ \leftrightarrow \cdots - Sn - O - m - R \tag{25}$$

Equations 23, 24 and 25 are equilibrium reaction. For this reason, the catalyst can also be deactivated and not only activated. Octanoic acid is produced as by-product of the catalyst activation. [3]

The ring opening polymerization is happening via a coordination-insertion mechanism. The Sn (II) alcoxide metal coordinates temporarily with the carbonyl group of the lactide by increasing the alcoxide nucleophilicity and the electrophility of the carbonyl group. Thus, the insertion of the monomer in the Sn-O bond is facilitated. Due to the active species and the catalyst and co-catalyst nature this coordination-insertion polymerization can be classified as an ionic polymerization followed by a step of monomer addition for the polymer chain growth. [8] Figure 5 shows the mechanism of coordination-insertion between the monomer and the catalyst.

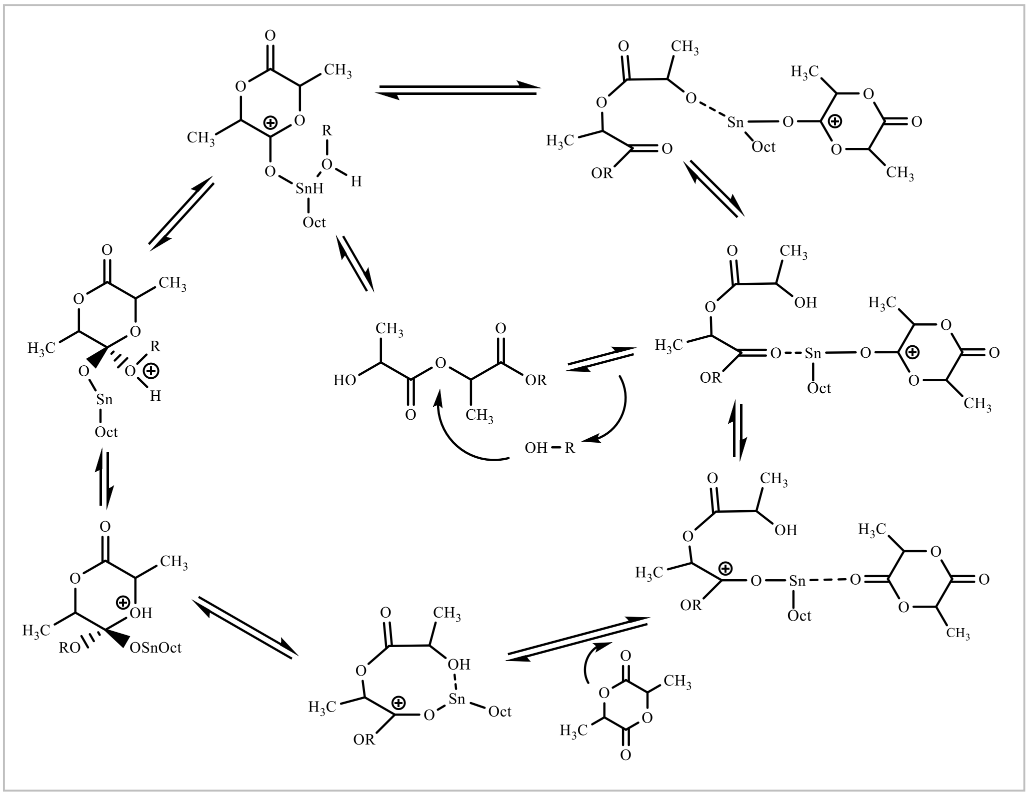


Figure 5. Coordination-insertion mechanism of lactide polymerization. [8]

2.3.2 Amount of catalyst and co-catalyst requirements

Although the equipment to be design is the reactor R-502, the catalyst must be introduced in the reactor R-301 and the reaction takes place in reactor R-501 and R-502. The amount of catalyst and co-catalyst depends on the required molecular weight of the final product, the temperature of operation, the residence time and the final conversion. The higher the amount of catalyst, the lower the residence time and the molecular weight. The higher the amount of co-catalyst, the lower the molecular weight and the time. However, if the amount of co-catalyst is too low, the initiation of the polymerization reaction cannot be considered enough faster and cannot be negligible for the simplification of further calculations. The figure 6 illustrates how the time of polymerization and the molecular weight depend on the concentration of catalyst and co-catalyst with respect the concentration of the monomer.

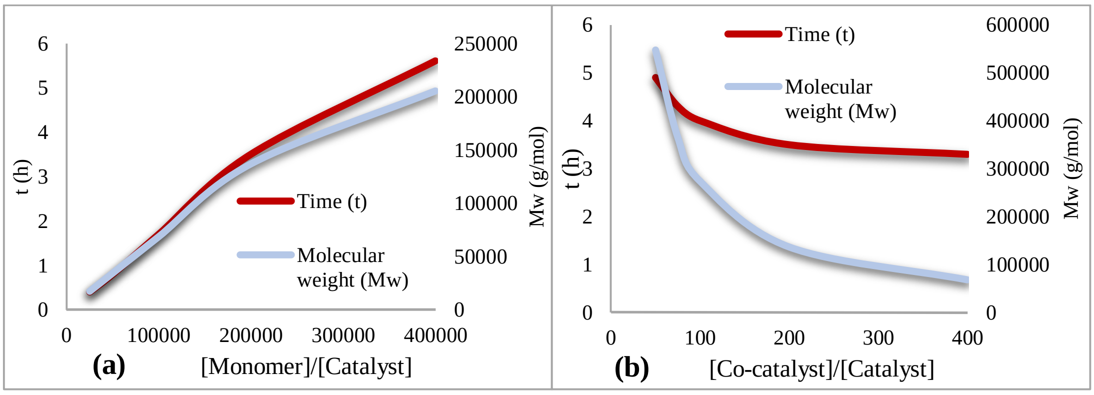


Figure 6. Monomer, catalyst and co-catalyst relationship with time and molecular weight for a 0.95 conversion of the monomer. (Own authorship).

In figure 6 the conversion has been set to 0.95. Figure 6.a has a fixed concentration relationship between co-catalyst and catalyst of 200 and figure 6.b has a fixed concentration relationship between the monomer and the catalyst of 200000. Under these conditions the poly (lactic acid) will have a 136970 g/mol at the outlet of reactor R-302 and a residence time of 3 h.

The final concentration of the catalyst can be calculated in agreement with equation 26.

$$[C] = \frac{-B + \sqrt{B^2 + 4\,[C]_0\,\left(K_{eq,a} - 1\right)([C]_0 + [A]_0)}}{2\,(K_{eq,a} - 1)} \tag{26}$$

Where,

$B = [A]_0 + 2\,[C]_0 + K_{eq,a}\,([S]_0 - [C]_0)$.

$K_{eq,a}$ = Equilibrium constant for the catalyst activation.

Table 4. Data and results for the amount of catalyst and co-catalyst needed.

Property	Value
$[M]_0$ (mol/l)	8.14
$[C]_0$ (mol/l)	4.07E-05
[C] (mol/l)	5.56E-06
$[A]_0$ (mol/l)	2.93E-04
$[S]_0$ (mol/l)	8.14E-03
[S] (mol/l)	8.10E-03
Catalyst (kg/h)	0.084
Co-catalyst (kg/h)	7.565

2.4 Dimension of the reactor- Volume

The design equation for an ideal plug flow reactor is described according to equation 27.

$$F_{A0}\frac{dx}{dV} = -r_A \qquad (27)$$

Where,

F_{A0} = Molar flow rate of the limiting reagent.

x = Conversion.

V = Volume of the reactor.

$-r_A$ = Reaction rate.

Although the plug flow behaviour might not be ideal, for simplification of calculations the reactor volume will be determined taking into account this assumption. The volume of this reactor has been calculated with equation 28, which has been deduced from equations 17, 19 and 27.

$$V = F_{M0}\int_{x_{in}}^{x_{out}} \frac{dx}{k_p\,[R^*]\,[M] - k_d\,[R^*]} \qquad (28)$$

Where,

F_{M0} = Molar flow rate of the monomer (kmol/h).

x_{in} = Input conversion.

x_{out} = Output conversion.

2.5 R-502 reactor thermal design

2.5.1 Heat load and utility mass flow estimation

The heat load has been estimated from energy balances from the heat of the reaction in the reactor. Equation 29 is required for the estimation of mass flow rate of the utility need for refrigeration of the reactor.

$$Q = M_c C_{p,c}(T_{c,o} - T_{c,i}) \tag{29}$$

Where,

Q = Heat load (W).

M_c = Mass flow rate of the utility (kg/s).

$C_{p,c}$ = Heat capacity of the utility (J/kg ºC).

$T_{c,o}$ = Outlet temperature of the utility (ºC).

$T_{c,i}$ = Intlet temperature of the utility (ºC).

2.5.2 Estimation of the log mean temperature difference

The log mean temperature difference can be estimated for countercurrent flow with equation 30.

$$LMTD = \frac{\left(T_{h,i} - T_{c,o}\right) - (T_{h,o} - T_{c,i})}{\ln[\,(T_{h,i} - T_{c,o})/(T_{h,o} - T_{c,i})]} \tag{30}$$

Where,

$T_{h,i}$ = Inlet temperature of the process fluid (ºC).

$T_{h,o}$ = Outlet temperature of the process fluid (ºC).

2.5.3 Calculation of heat transfer area

The heat transfer area is calculated with equation 31.

$$A_o = \frac{Q}{U\ F\ LMTD} \tag{31}$$

Where,

U = Overall heat transfer coefficient (W/m^2 ºC).

F= Temperature correction factor.

The correction factor is equal to 1 for this heat transfer equipment because has a single tube pass and the flow is in countercurrent.

2.5.4 Determination of the number of tubes

The number of tubes can be calculated from equation 32.

$$A_o = \pi d_o L_{ta} N_t \tag{32}$$

Where,

d_o= Outer diameter of the tubes (m).

L_{ta}= Tube length (m).

N_t = Number of tubes.

2.6 R-502 reactor mechanical design

2.6.1 Design code specification

The reactor R-502 has been design in agreement with the TEMA standards and the ASME Code Section VIII, Division 1.

The TEMA standards are applicable for shell and tube heat exchangers, just like the configuration shown for Reactor R-502, with maximum design pressures of 20684.27 kPa (3,000 psi), a maximum inside diameter of the shell of 1524 mm (60 in), a maximum wall thickness of the shell of 50.8 mm (2 in) and a maximum tube thickness of 76.2 mm (3 in). Although reactor R-502 is expected to have a larger inside diameter of the shell, the criteria of the TEMA standards can also be applied.

The Division 1 of the ASME Code section VIII can be applied with external and internal design pressures over 100 kPa (15 psi) and lower than 20684.27 kPa (3,000 psi). As the design pressure is higher than 100 kPa, the ASME code also applies to these design.

2.6.2 Type of TEMA design

The TEMA standard describes the shell and tube heat exchanger configuration in agreement with three main components: front head, shell section and rear head.

There are seven types of shells which are codified with different letters: One-pass shell (E), two-pass shell (F), Split flow (G), Double split flow (H), divided flow (J), Kettle type reboiler (K) and crossflow (X). The most suitable shell for reactor R-502 is the one-pass shell.

Reactor R-502 has also a floating head configuration, which mainly consists of a stationary tubesheet and a floating tubesheet. There are four types of floating heads but the one chosen for the equipment to be design is the floating head with externally sealed floating tubesheet. This head is the cheapest floating head, operates at low pressures and the tube bundle is removable for cleaning operations. The nomenclature for this head is W and can be used with A, B and C front heads.

Summarizing, the TEMA designation for reactor R-502 is BEW.

2.6.3 Design temperature and pressure

The design temperature is the maximum operating temperature of the equipment plus 50 ºF. For these reason, for an operating temperature of 180ºC, the design temperature is 207.78ºC.

$$T_{design} = (180^{o}C \cdot 1.8 + 32)\ °F + 50\ °F = 406\ °F = 207.78\ °C$$

The vessels or other equipment under external pressure (for example vacuum) must be design to bear with the maximum pressure difference during operation. For this reason, the external design pressure can be estimated as the difference between the atmospheric pressure or pressure at the outside of the shell and the maximum vacuum pressure at the inside of the vessel. The worst condition in the inside of the vessel is the full vacuum.

$$P_{desing} = -101.325\ kPa$$

2.6.4 Selection of materials for mechanical design construction

The selection of the materials for the construction of the reactor R-502 has been made in agreement with the Ashby methodology, which is a graphic method for the optimization of the design process selection of a material as a function of the material properties, geometric parameters and functional requirements. This method can only be used as approximation and is not used for more detailed designs. The design requirements taken into account for the material selection are summarized in table 5.

Table 5. Design requirements for material selection. (Own authorship)

Function	Chemical reactor with heat exchange (design as a heat exchanger).
Constraints	Support pressure difference. Operating temperature up to 180ºC. Withstand the lactide and PLA chemical and physical properties. Economics: Modest cost.
Objectives	Withstand with low pressures (vacuum). Maximize heat flow per unit area.
Free variables	Choice of material.

The reactor R-502 is a pressure vessel submitted to external pressure and high temperatures. The selection of the materials is made in accordance with figures 7, 8, 9 and 10. Material indexes are required for figures 7 and 8. The heat flow per unit area of the tube wall is increased for the materials indicated, in figure 7, above the line drawn from the material index expressed as $M = \sigma_y \lambda$.

A leak-before-break criterion is used for safety in large pressure vessels. Moreover, the economy of the material must be considered. In agreement with these two reasons, the material indexes $\mathrm{M_3} = {}^{\mathrm{K_{1c}^2}}/_{\sigma_\mathrm{f}}$ and $M_4 = \sigma_f$ must be maximize in figure 8.

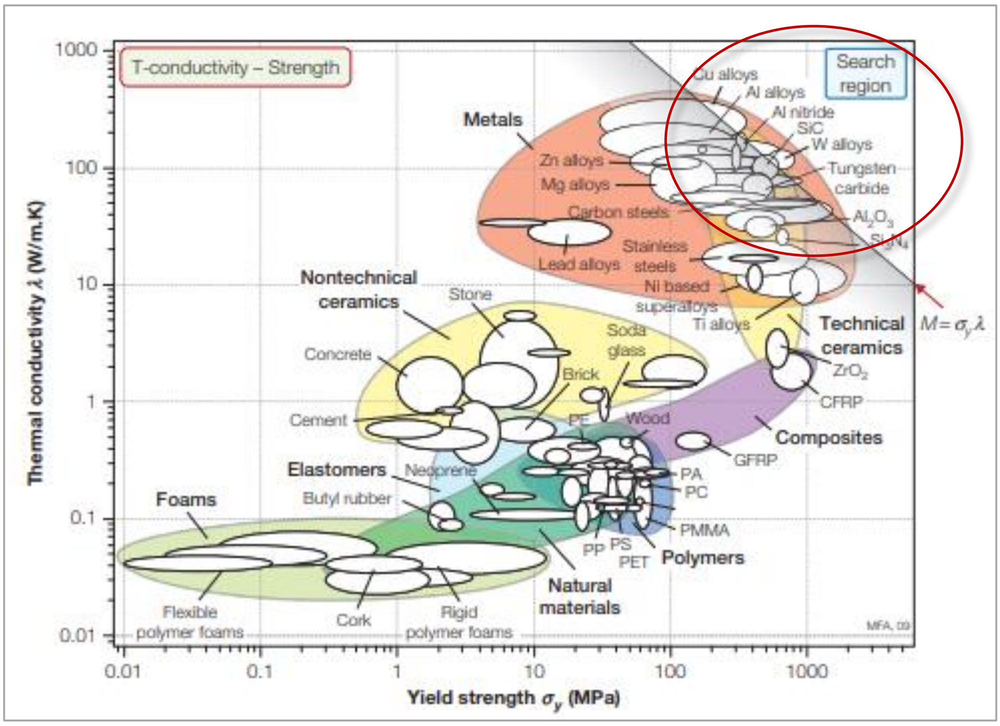


Figure 7. Yield strength against thermal conductivity chart. [9]

In general, the metals groups have the greatest thermal conductivity and fracture toughness.

Figures 9 and 10 show different types of materials in agreement with its temperature of operation and price. In this case, there are a wide range and groups of materials to be considered.

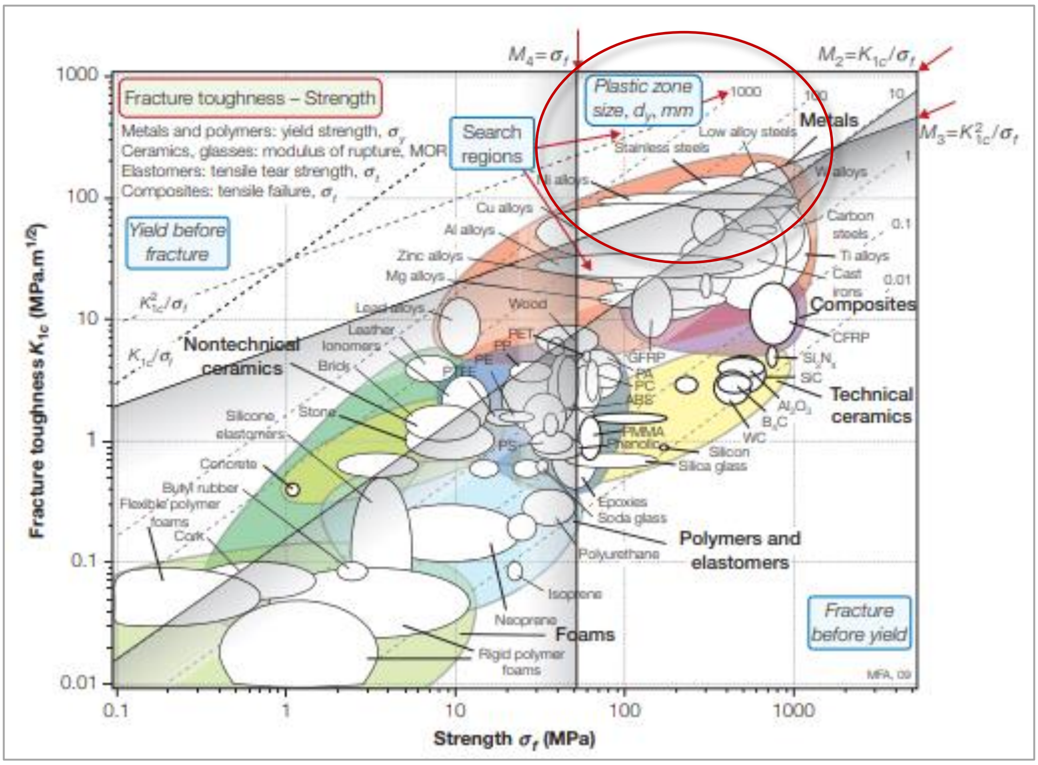


Figure 8. Fracture toughness against strength. [9]

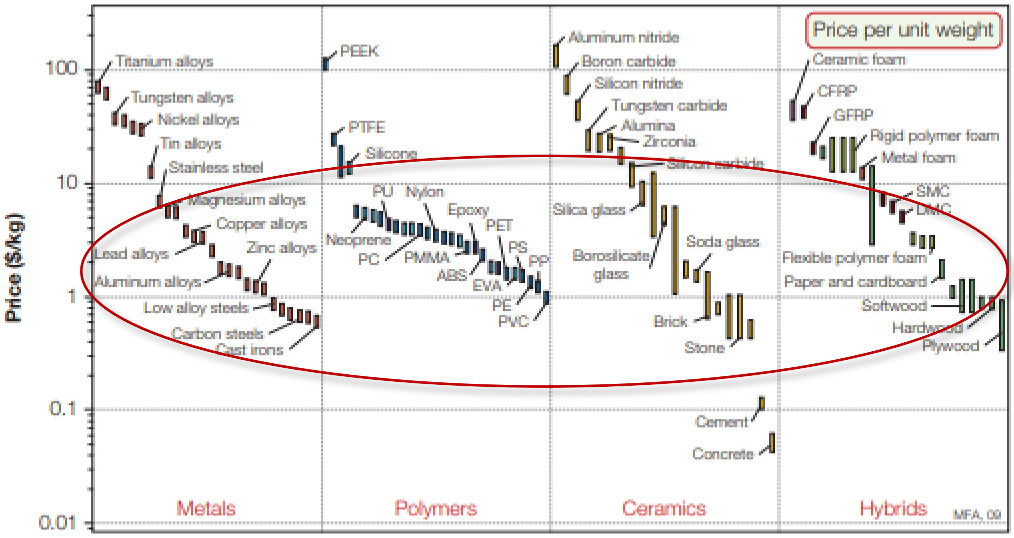


Figure 9. Approximate price per kilogram of material. [9]

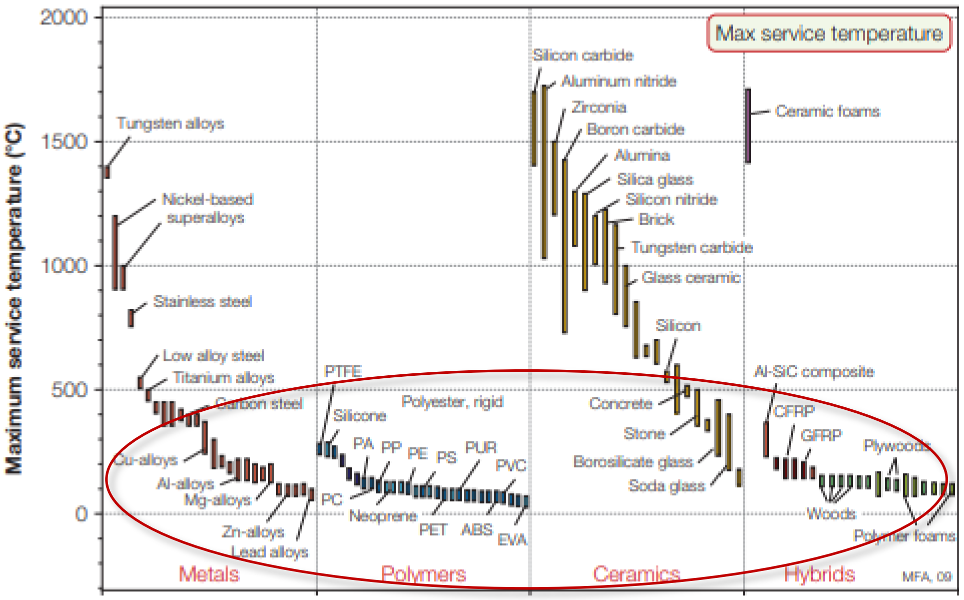


Figure 10. Maximum temperature of operation for different materials. [9]

Before the selection of the construction material is indicated, other characteristics like the corrosivity of the materials to be processed in the reactor must be analysed. Although PLA and lactide are not a corrosive materials, lactic acid is very corrosive. Reactor R-502 transforms lactide to PLA and is expected to be free of water and lactic acid. However, a complete 100% separation is not possible and traces of these materials can be found.

In accordance to the information given above, the construction material to be selected is stainless steel 316.

2.6.5 Detailed mechanical design

2.6.5.1 Introduction

The reactor R-502 has been design as a shell and tube heat exchanger in agreement with the Bell-Delaware Method. This method assumes that the following data for the shellside is already given: density, viscosity, thermal conductivity, specific heat and inlet and outlet temperatures. [11]

2.6.5.3 Input data

Initially, all the geometrical parameters indicated above must be assumed: [11]

1. Outside diameter of the tubes.
2. Layout pattern of the tubes.

3. Baffle cut.
4. Central baffle spacing.
5. Inside diameter of the shell.
6. Number of the sealing strips per side.

2.6.5.4 Shellside and tubeside fluid allocation

The location of the process fluid and the utility required for refrigeration of the reactor were chosen taking into account some of the following factors: corrosion, fouling, cleanability, temperature, pressure, pressure drop, viscosity, flow rate and toxicity of fluids.

One more aspect should be considered for the allocation of the fluids: the volume required for reaction. Reactor R-502 is design as a heat exchanger and, accordingly, this consideration is important when sizing the equipment.

The process fluid (mixture of lactide and PLA) has been routed through the shellside and the refrigeration fluid (water) flows through the tubes. The explained allocation has been considered due to:

1. If the water is located in the shellside (and due to the flow rate of water required for heat removal is not very high), the velocity of water would be considerably low. Very small tube diameters in the heat exchanger would be required for higher velocities.
2. The viscosity of the reactant mixture produces a high pressure drop if located in small tubes. Moreover, the heat transfer rates are smaller than those for the process fluid inside the shellside.
3. When the process fluid is inside tubes, the volume of reaction would require small tubes with a large shell diameter and length or tubes with higher diameter (which reduces the velocity of water in the shellside).

In addition to the previously explained and in order to increase the heat transfer, both fluids would be in countercurrent flow.

2.6.5.5 Shell side calculation parameters

Some calculations for the shell side are explained in this section. Figure 11 gives an idea of the parameters to be estimate for the shellside.

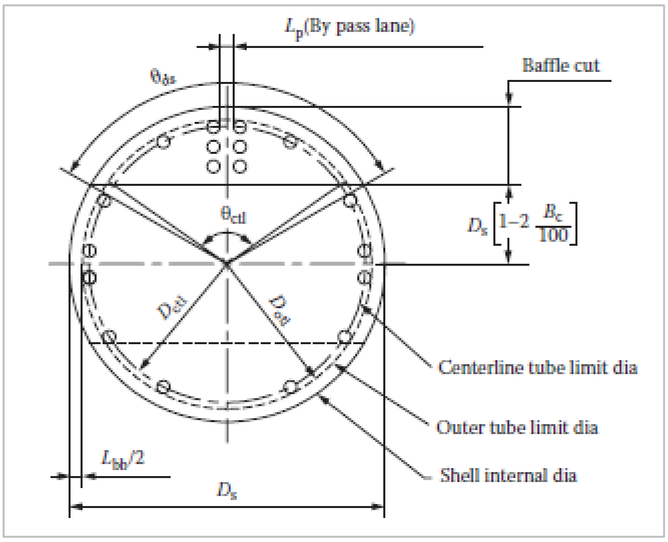


Figure 11. Drawing of a cut of the shellside diameter components. [11]

The bundle to the shell clearance can be estimated with the linear function shown in equation 33, specified by TEMA standards.

$$L_{bb} = 12.0 + 0.005\ D_s \tag{33}$$

Where,

L_{bb} = Bundle to shell clearance (mm).

D_s = Inside diameter of the shell (mm).

The diameter of the bank of tubes can be estimated with equation 34 and the bundle diameter with equation 35.

$$D_{otl} = D_s - L_{bb} \tag{34}$$

$$D_{ctl} = D_{otl} - d_o \tag{35}$$

Where,

D_{otl} = Outer diameter limit of the tube bank (mm).

D_{ctl} = Diameter of the bundle of tubes (mm).

The geometry of the baffle in relation to the tube bank can be described with the following two parameters: the centriangle of the baffle cut and the upper centriangle of the baffle cut. Both are angles obtained from the intersection of the baffle cut with the inside wall of the shell and the diameter of the bundle of tubes, respectively.

$$\theta_{ds} = 2cos^{-1}\left(1 - \frac{2\ B_c}{100}\right) \tag{36}$$

$$\theta_{ctl} = 2cos^{-1}\left[\frac{D_s}{D_{ctl}}\left(1-\frac{2\,B_c}{100}\right)\right] \tag{37}$$

Where,

θ_{ds} = Centriangle of baffle cut (rad).

θ_{ctl} = Upper centriangle of the baffle cut (rad).

B_c = Baffle cut (%).

The tube length assumption is very important when describing the geometry of the equipment. However, there are other measurements to be calculated for the fully definition of the shellside.

Figure 12 shows schematically some significant lengths. Nevertheless, the outer tube bend radius is not considered for the reactor because the configuration is not U-tube.

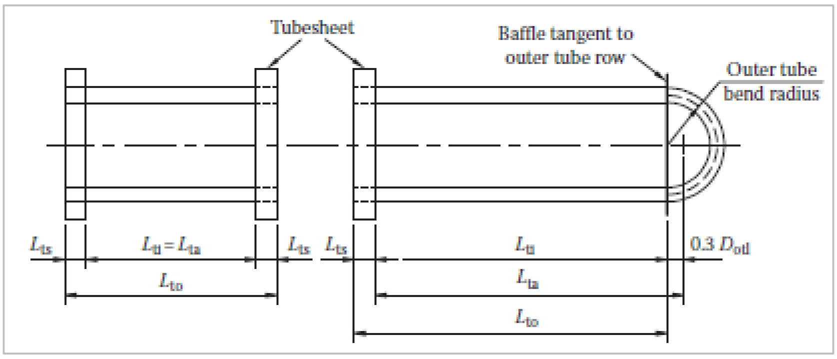


Figure 12. Significant lengths of the shell and tube heat exchanger configuration. [11]

The shell length is calculated with equation 38.

$$L_{to} = L_{ta} + 2\,L_{ts} \tag{38}$$

Where,

L_{ta} = Tube length (mm).

L_{ts} = Thickness of the tubesheet (mm).

The thickness of the tubesheet is assumed to be 25.4 mm and the space between the tube walls, defined as bypass lane partition is assumed to be $L_p = d_o$.

Regarding to the tubes, figure 13 illustrates some other parameters for the definition of tube layout and spaces among them.

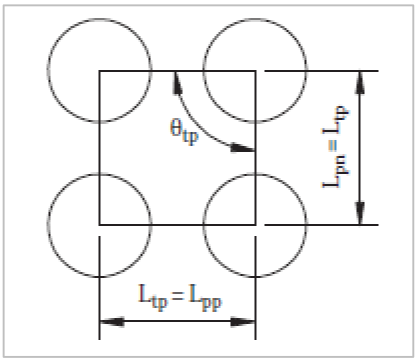


Figure 13. Parameters of a tube layout of 90º.

For a layout pattern of the tubes, θ_{tp}, of 90º equations 39, 40 and 41 indicates the calculation of the tube pitch, the effective tube pitch and the effective tube row distance.

$$L_{tp} = 1.25\ d_o \tag{39}$$

$$L_{tp,eff} = L_{tp} \tag{40}$$

$$L_{pp} = L_{tp} \tag{41}$$

The number of baffles can be estimated with equation 42.

$$N_b = \frac{L_{ta}}{L_{bc}} - 1 \tag{42}$$

Where,

L_{bc} = Central baffle spacing (mm).

The number of effective tube rows in the total shell, the number of tube rows in the baffle window and the number of tubes in the window were calculated in agreement with equations 43, 44 and 45.

$$N_{tcc} = \frac{D_s}{L_{pp}}(1 - \frac{2\ B_c}{100}) \tag{43}$$

$$N_{tcw} = \frac{0.8}{L_{pp}}\left[\frac{D_s B_c}{100} - \frac{D_s - D_{ctl}}{2}\right] \tag{44}$$

$$N_{tw} = N_t F_w \tag{45}$$

Where,

F_w = Fraction of the tubes number in the baffle window.

The fraction of tubes can be estimated following the equation 46.

$$F_w = \frac{\theta_{ctl}}{2\pi} - \frac{\sin\theta_{ctl}}{2\pi} \tag{46}$$

Finally the geometry of the equipment can be defined with the indication areas named aboved.

1. Crossflow area of the shellside at the bundle centerline.

$$S_m = L_{bc}\left[L_{bb} + \frac{D_{ctl}}{L_{tp,eff}}\left(L_{tp} - d_o\right)\right] \tag{47}$$

2. Flow area in the baffle window.

$$S_{wg} = \frac{\pi}{4}D_s^2\left(\frac{\theta_{ds}}{2\pi} - \frac{\sin\theta_{ds}}{2\pi}\right) \tag{48}$$

3. Flow area of the baffle window with tubes.

$$S_{wt} = N_{tw}\frac{\pi}{4}d_o^2 \tag{49}$$

4. Net crossflow area in the baffle window.

$$S_w = S_{wg} - S_{wt} \tag{50}$$

5. Bypass area between shell and bundle.

$$S_b = L_{bc}\,(D_s - D_{otl} + L_p) \tag{51}$$

6. Leakage area between the shell and the baffle.

$$S_{sb} = \pi D_s\frac{L_{sb}}{2}\left(\frac{2\pi - \theta_{ds}}{2\pi}\right) \tag{52}$$

7. Hole of the leakage area between the tube and the baffle.

$$S_{tb} = \frac{\pi}{4}\,[(d_o + L_{tb})^2 - d_o^2]N_t\,(1 - F_w) \tag{53}$$

2.6.5.6 Shellside heat transfer coefficient

The heat transfer coefficient for the shellside can be estimated for Bell-Delaware method with the correction of the ideal heat transfer coefficient in crossflow. [11]

$$h_s = h_i J_c J_1 J_b J_s J_r \tag{54}$$

Where,

h_s = Heat transfer coefficient of the shell side (W/m^2 ºC).

h_i = Heat transfer coefficient for the ideal bank of tubes (W/m^2 ºC).

J_c = Correction factor for heat transfer for baffle window.

J_1 = Correction factor for heat transfer due to leakage effects in the baffle.

J_b = Correction factor for heat transfer due to the bypass flow in the bundle of tubes.

J_s = Correction factor for heat transfer due to the baffle spacing in input and output.

J_r = Correction factor for heat transfer due to extreme temperatures.

The correction factor for the effects of the flow in baffle window can be calculated with equation 55. This value must be approximately 1 when the heat exchanger works with liquid in the shellside.

$$J_c = 0.55 + 0.72\ F_c \tag{55}$$

Where,

F_c = Fraction of tubes in pure crossflow.

F_c can be calculated once the fraction of the number of tubes in the baffle window (F_w) is already known.

$$F_c = 1 - 2\ F_w \tag{56}$$

The correction factor J_1 establishes a comparison between the leakage streams and the crossflow streams and specifies when the baffles were placed too close. The optimum range is 0.7-0.9 for this correction factor.

$$J_1 = 0.44\ (1 - r_s) + [1 - 0.44\ (1 - r_s)]e^{-2.2\ r_{lm}} \tag{57}$$

Where,

$$r_s = \frac{S_{sb}}{S_{sb} + S_{tb}} \tag{58}$$

$$r_{lm} = \frac{S_{sb} + S_{tb}}{S_m} \tag{59}$$

The correction factor due to the bypass flow in the bundle of tubes can be estimated with equation 60. This factor should have a value around 0.9 for small shell-bundle tube clearances.

$$J_b = exp\{-C_{bh}F_{sbp}[1 - (2r_{ss})^{1/3}]\} \tag{60}$$

Where,

$$F_{sbp} = \frac{S_b}{S_m} \tag{61}$$

$$r_{ss} = \frac{N_{ss}}{N_{tcc}} \tag{62}$$

$$C_{bh} = 1.25 \tag{63}$$

Correction factor due to the baffle spacing in input and output can be calculated with equations 64, 65 and 66. This factor has its optimum value in a range 0.85-1. A relationship of $L_{bi} = L_{bo} = [L_{ti} - (N_b - 1)]/2$ has been considered the reactor design.

$$J_s = \frac{(N_b - 1) + (L_i^*)^{1-n} + (L_o^*)^{1-n}}{(N_b - 1) + \left(L_i^* - 1\right) + (L_o^* - 1)} \tag{64}$$

$$L_i^* = \frac{L_{bi}}{L_{bc}} \tag{65}$$

$$L_o^* = \frac{L_{bo}}{L_{bc}} \tag{66}$$

Where,

L_{bi} = Inlet baffle spacing.

L_{bo} = Outlet baffle spacing.

n = Value of 1 for laminar flow.

Correction factor due to extreme temperatures must be calculated for laminar flow, which is the particular case of this design. For $Re_s < 20$, the correction factor is calculated with equations 67 and 68.

$$J_r = \frac{1.51}{N_c^{0.18}} \tag{67}$$

$$N_c = (N_{tcc} + N_{tcw})(N_b + 1) \tag{68}$$

Finally, the ideal heat transfer coefficient is calculated with,

$$h_i = \frac{j_i C_{ps} G_s (\emptyset_s)^n}{Pr_s^{2/3}} \tag{69}$$

Where,

j_i = Ideal Colburn factor.

C_{ps} = Heat capacity on the shellside (J/kg ºC).

G_s = Mass velocity in the shellside (kg/m^2 s)

$(\emptyset_s)^n$ = Viscosity correction factor.

Pr_s = Prandtl number in the shellside.

The Prandtl number, the mass velocity in the shellside and the Reynolds number in the shellside are given by equations 71, 72 and 73.

$$Pr_s = \frac{\mu_s C_{ps}}{k_s} \tag{70}$$

$$G_s = \frac{M_s}{S_m} \tag{71}$$

$$Re_s = \frac{D_w G_s}{\mu_s} \tag{72}$$

Where,

μ_s = Viscosity in the shellside (kg/m s).

k_s = Thermal conductivity of the shellside fluid (W/m ºC).

M_s = Mass flow rate in the shellside (kg/s).

D_w = Hydraulic diameter of the shellside (m).

The hydraulic diameter of the shellside can be estimated in agreement with equation 73.

$$D_w = \frac{4S_w}{\pi d_o N_{tw} + \pi D_s \theta_{ds}/2\pi} \tag{73}$$

The ideal Colburn factor can be estimated with equations 74 and 75. [12]

$$j = a_1 \left(\frac{1.33}{L_{tp}/d_o} \right)^a (Re_s)^{a_2} \tag{74}$$

$$a = \frac{a_3}{1 + 0.14\,(Re_s)^{a_4}} \tag{75}$$

Where, a_1, a_2, a_3 and a_4 are constants depending on the Reynolds number on the shellside and the layout angle of the tubes. For $Re_s < 10$ and a tube layout of 90º, the values for the constants are 0.97, -0.667, 0 and 0, respectively.

2.6.5.7 Shell side pressure drop

The total pressure drop in the shellside is given by,

$$\Delta p_s = \Delta p_c + \Delta p_w + \Delta p_e \tag{76}$$

Where,

Δp_c = Pressure drop due to crossflow (Pa).

Δp_w = Pressure drop due to the window regions (Pa).

Δp_e = Pressure drop due to the inlet and outlet regions (Pa).

The pressure drop elements of the equation 76 are related to the region in the shellside according to figure 14.

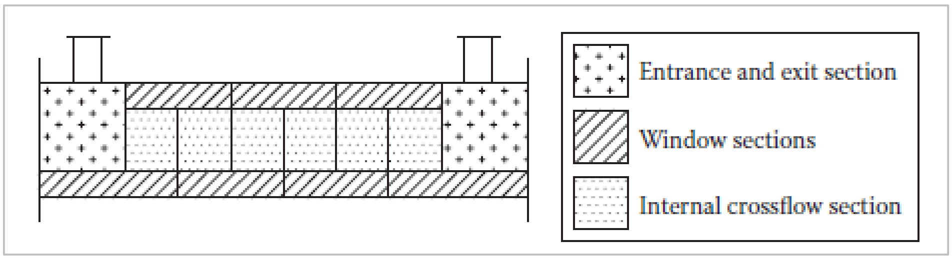


Figure 14. Regions for the pressure drop in the shellside. [11]

The pressure drop for the crossflow section is estimated with equation 77.

$$\Delta p_c = (N_b - 1)(\Delta p_{b,i} R_b R_1) \tag{77}$$

Where,

$\Delta p_{b,i}$ = Pressure drop in the ideal tube bank (Pa).

R_b = Correction factor for pressure drop due to the bypass flow in the bundle of tubes.

R_1 = Correction factor for pressure drop due to leakage effects in the baffle.

The correction factors of equation 77 can be estimated in agreement with,

$$R_b = e^{\{-C_{bp}F_{sbp}[1-(r_{ss})^{1/3}]\}} \tag{78}$$

$$R_1 = \exp[\,-1.33\,(1 + r_s)]\, r_{lm}^{x} \tag{79}$$

$$x = [-0.15\,(1 + r_s) + 0.8] \tag{80}$$

The pressure drop in the ideal tube bank must be estimated with equation 81.

$$\Delta p_{b,i} = 2 f_s N_{tcc} \frac{G_s^2}{g_c \rho_s} (\emptyset_s)^{-n} \tag{81}$$

Where,

f_s = Friction factor.

ρ_s = Density of the fluid in the shellside (kg/m^3).

The ideal Colburn factor can be estimated with equations 82 and 83. [12]

$$f = b_1 \left(\frac{1.33}{L_{tp}/d_o}\right)^{b} (Re_s)^{b_2} \tag{82}$$

$$a = \frac{b_3}{1 + 0.14\,(Re_s)^{b_4}} \tag{83}$$

Where, b_1, b_2, b_3 and b_4 are constants depending on the Reynolds number on the shellside and the layout angle of the tubes. For $Re_s < 10$ and a tube layout of 90º, the values for the constants are 35, -1, 0 and 0, respectively.

Pressure drop due to the window regions is estimated with equation 84 for $Re_s < 100$.

$$\Delta p_w = 26\, \frac{G_w \mu_s}{g_c \rho_s} \left(\frac{N_{tcw}}{L_{tp} - d_o} + \frac{L_{bc}}{D_w^2}\right) + 2 \frac{G_w^2}{g_c \rho_s} \tag{84}$$

Where,

$$G_w = \frac{M_s}{\sqrt{S_m S_w}} \tag{85}$$

Where,

G_w = Window mass velocity (kg/m^2 s).

Finally, the pressure drop due to the inlet and outlet regions is given by,

$$\Delta p_e = 2(\Delta p_{b,i}) \left(1 + \frac{N_{tcw}}{N_{tcc}}\right) R_b R_s \tag{86}$$

Where,

R_s = Correction factor for the pressure drop due to the baffle spacing in input and output.

The correction factor due to inlet and outlet pressure drop is given by equation 87.

$$R_s = \left(\frac{1}{L_i^*}\right)^{2-n} + \left(\frac{1}{L_o^*}\right)^{2-n} \qquad (87)$$

The velocity in the shellside is estimated as,

$$v_s = \frac{M_s}{\rho_s S_m} \qquad (88)$$

2.6.5.8 Tube side heat transfer coefficient

The heat transfer coefficient on the tubeside is calculated from,

$$\frac{h_t d_i}{k_t} = j_h Re_t {Pr_t}^{0.33} \qquad (89)$$

Where,

Re_t = Reynolds number in the tubeside.

Pr_t = Prandtl number in the tubeside.

d_i= Inside diameter of the tubes (m).

k_t = Thermal conductivity of the tubeside fluid (W/m ºC).

j_h = Heat transfer factor of the tube side.

The heat transfer factor can be estimated with figure 15.

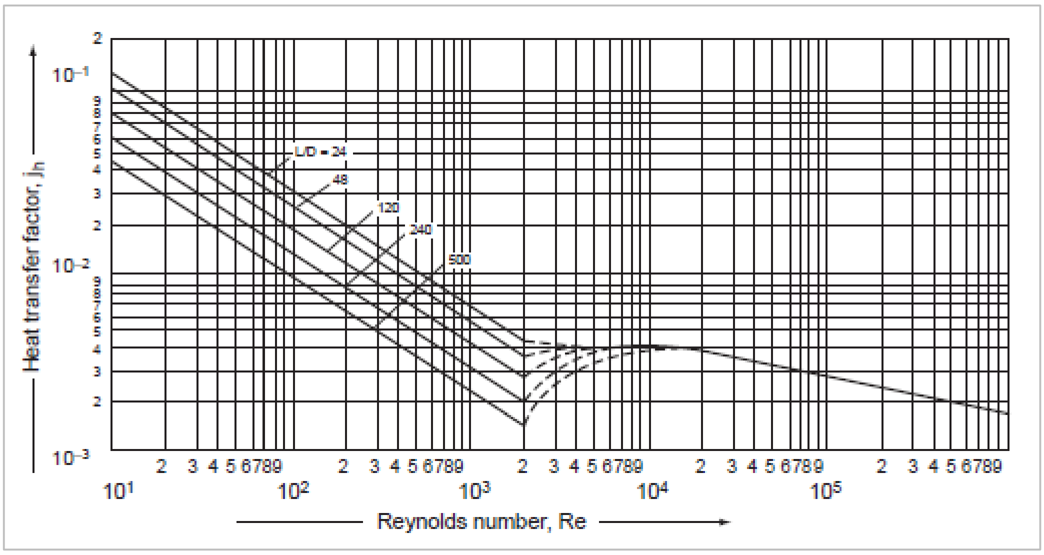


Figure 15. Heat transfer factor in the tubeside. [13]

The Reynolds number and the Prandtl number for the tubeside can be calculated with equations 91 and 92.

$$Re_t = \frac{G_t d_i}{\mu_t} \tag{90}$$

$$Pr_t = \frac{\mu_t C_{pt}}{k_t} \tag{91}$$

Where,

G_t = Tubeside mass velocity (kg/m^2 s).

μ_t = Viscosity of the fluid in the tubeside (kg/m s).

C_{pt} = Heat capacity of the fluid in the tubeside (J/kg ºC).

The tubeside mass velocity is calculated from the mass flow rate and the flow area of the tubeside.

$$G_t = \frac{M_t}{A_t} \tag{92}$$

$$A_t = \frac{\pi}{4} d_i^2 N_t \tag{93}$$

2.6.5.9 Tube side pressure drop

The tubeside pressure drop for the reactor can be calculates in agreement with equation 95. This equation considers the pressure drop due to friction losses in the tubes in the first term and the losses due to sudden contraction and expansion in the second term. This equation is applied because the fluid is not viscous and the number of passes per pass is one.

$$\Delta p_t = \left[8 j_f \left(\frac{L}{d_i}\right) + 2.5\right] \frac{\rho v_t^2}{2} \tag{94}$$

Where,

j_f = Friction factor in the tubeside.

The friction factor for commercial heat exchanger tubes with a turbulent flow is calculated as: [12]

$$j_h = 0.4137\ Re_t^{-0.2585} \tag{95}$$

The velocity in the tubeside is estimated as,

$$v_t = \frac{M_t}{\rho_t A_t} \tag{96}$$

2.6.5.10 Estimation of the overall heat transfer coefficient.

The overall heat transfer coefficient is given by,

$$U = \frac{1}{[(1/h_s) + R_{fo} + (t_w/k_w)(r_o/(r_o + r_i)) + \left(R_{fi} + (1/h_t)\right) r_o/r_i]} \tag{97}$$

Where,

t_w = Tube thickness (m).

R_{fo} = Fouling resistance of the shellside (m^2 ºC/W).

R_{fi} = Fouling resistance of the tubeside (m^2 ºC/W).

k_w = Wall resistance (W/m ºC).

r_o = Tube outer radius (m).

r_i = Tube inner radius (m).

The fouling resistances can be assumed within a certain range in agreement with the information provided in table 6.

Table 6. Typical fouling resistances. [14]

	$^1/_{R_{fo}}$ ***and*** $^1/_{R_{fi}}$ **(W/m^2 ºC)**
Water	
Distilled	11,000
Boiler feedwater	6,000-11,000
Town water	2,000-5,000
Well water	1,000-3,000
Clear river	2,000-6,000
Good-quality cooling water	3,000-6,000
Poor-quality cooling water	1,000-2,000
Sea	6,000-1,000
Boiler blowdown	3,000
Steam	
Good quality	20,000
Contaminated	5,000-11,000
Liquids	
Aqueous salt solutions	3,000-6,000
Organic (low viscosity)	3,000-11,000
Organic (high viscosity)	1,000-3,000
Machinery oil	6,000
Fuel oils	1,000
Tars	500-1,000
Vegetable oils	2,000
Gases	
Air	2,000-4,000
Organic vapour	5,000-11,000

2.6.5.11 Well join efficiencies

Well joint efficiencies are described in subsection B part UW of the ASME code section VIII division 1. In agreement with the indicated information. The reactor R-502 will have the following well joint categories in different parts of the equipment.

- Category A: For the longitudinal welded joints in the shell.
- Category B: For circumferential welded joints in the shell.
- Category C: For the tubesheet and connections.
- Category D: For the connecting nozzles of the heat exchanger.

The joints of category A are going to be doubled welded butt joints. All butt well joints must be fully radiographed and in other cases the joints will not need a radiographic examination.

2.6.6 Minimum thickness of the Shell of the equipment

The ASME BPV code has a basic design for the calculation of the shell minimum thickness on its section VIII division 1. The equations required for this calculation must be appropriate for vessels submitted to external pressure because the shell side of the equipment is under vacuum pressure.

The thickness of the shell can be determined in agreement with the next procedure:

1. Expressed the internal vacuum pressure as external pressure.
2. Assume a thickness for the shell.
3. Calculate D_o/t, ratio between the outside diameter of the shell and the thickness.
4. Calculate L/D_o, ratio between the shell length and the outside diameter of the shell.
5. Enter figure 11 and estimate factor A.
6. Enter figure 12 with the factor A and the modulus of elasticity and estimate B.
7. Consider a safety design factor of 3 for the bulking of cylindrical shells.
8. Calculate the allowable pressure for the assumed thickness and compare it with the external pressure.

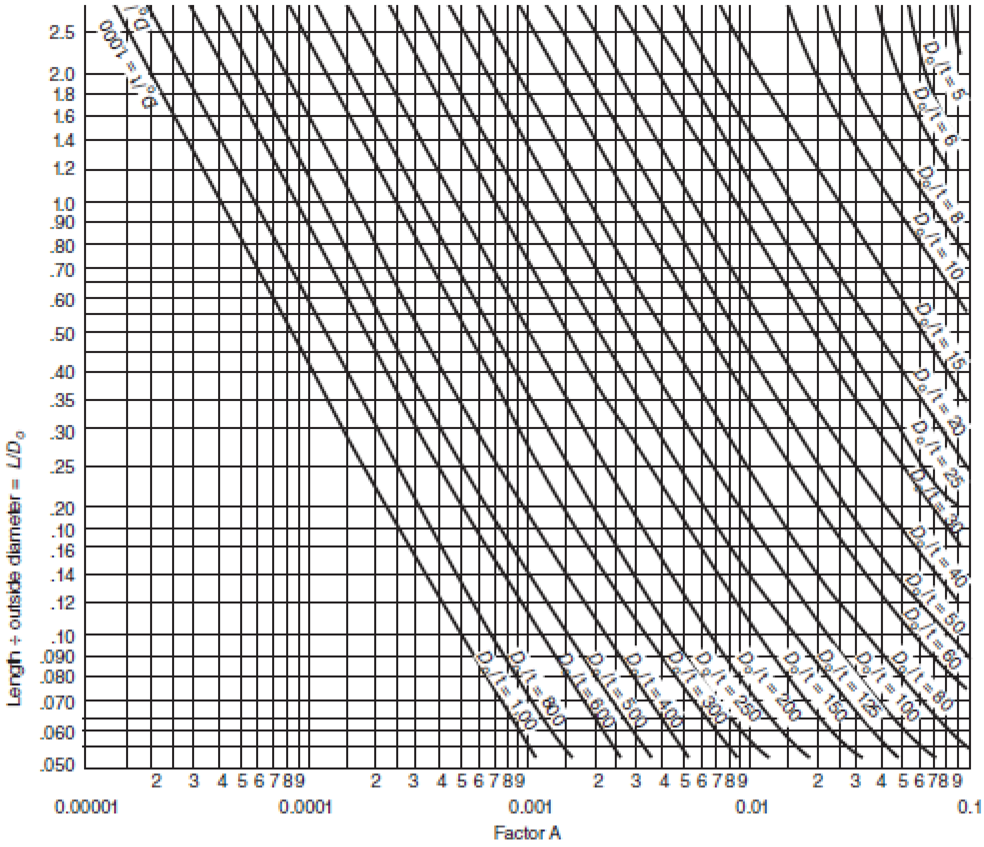


Figure 16. Chart for cylindrical vessels under external pressure. [10]

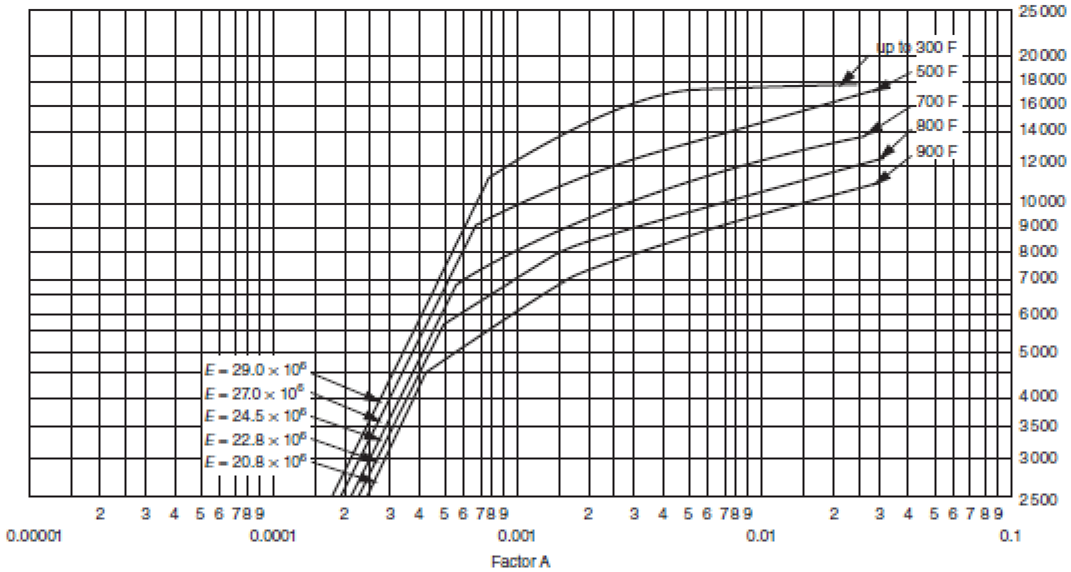


Figure 17. Chart for shell thickness determination for cylindrical vessels under external pressure. [10]

Factor B (expressed in psi) shown in figure 17 indicates whether the buckling is inside the elastic or inelastic region. In accordance, for $D_o/t \geq 10$ and inside the elastic region, the allowable pressure is calculated as indicated in equation 27.

$$P = \frac{2\,A\,E_0}{3\,(D_o/t)} \tag{98}$$

Where,

A = Factor from figure 16.

E_0 = Modulus of elasticity (kPa).

D_o = Outside diameter of the shell (m).

t = Thickness of the shell (m).

If $P_{allowable} \geq P_{external}$ the assumed thickness is acceptable.

2.6.7 Minimum thickness for heads and closures

There are different types of heads and closures: ellipsoidal, torispherical, hemispherical, toriconical, conical... The selection of one of them depends on the thickness required in order to bear with the pressure for the operation of the reactor. In this section the ellipsoidal, torispherical and hemispherical heads are analysed for pressure on the convex side (external pressure or vacuum). [15]

The procedure for the determination of the thickness is very similar in the three cases.

1. The procedure required is similar to the one used for the calculation of the thickness in spherical shells.
2. The thickness must be initially assumed.
3. Factor A can be calculated with equation 99.
4. Factor B can be determined with figure 17 for a specific material and temperature.
5. Once factor B is known, the allowable working pressure can be estimated with equation 100.
6. The procedure must be repeat again until, for the specified thickness, the allowable working pressure is greater than the design pressure.

Equations 99 and 100 are shown below.

$$A = \frac{0.125}{(R_o/t)} \tag{99}$$

$$P_a = \frac{B}{(R_o/t)} \qquad (100)$$

Where,

R_o = Different radius depending on the head type.

t = Thickness of the head or rear.

Ro is shell outside radius for hemispherical heads, is the equivalent outside spherical radius for ellipsoidal heads and is the outside radius of the crown for torispherical heads.

The equivalent outside spherical radius is defined as K_0D_0 where K_0 can be estimated from values in table 7 and h_0 is the length of the outside minor axis of the ellipsoidal head. This length is usually considered as 0.25 the inside diameter of the shell.

Table 7. K_o values for the equivalent diameter. [15]

$D_o/2h_o$	3.0	2.8	2.6	2.4	2.2	2.0	1.8	1.6	1.4	1.2	1.1
K_o	1.36	1.27	1.18	1.08	0.99	0.90	0.81	0.73	0.65	0.57	0.5

The outside radius of the crown is usually equal to the diameter of the shell.

The hemispherical head is the closure chosen for the reactor R-502 due to the obtained thickness for the design pressure. The configuration of a hemispherical head is shown in figure 18. The comparison between the results obtained for the analyzed heads is shown in table 17.

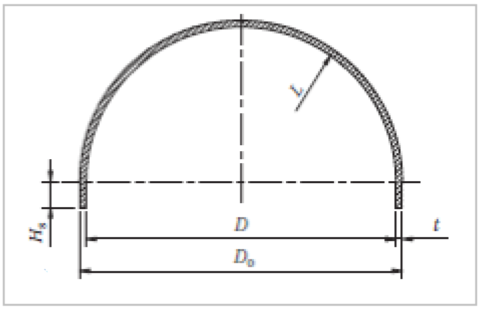


Figure 18. Hemispherical head configuration. [11]

2.6.8 Calculation of stresses

The shell of a heat exchanger can be considered as a thin cylindrical shell with external pressure. Although in a heat exchanger the shell is summited to other forces which are able to generate stresses, the radial and the hoop stresses are some of the most significant. Both can be calculated taking into account the previous assumption. [10]

The stress distribution for a cylinder submitted to external pressure can be estimated with equations 99 and 100.

$$\sigma_\theta = \frac{-P_o r_o^2}{r_o^2 - r_i^2} \left(\frac{r^2 + r_i^2}{r^2}\right) \tag{101}$$

$$\sigma_r = \frac{-P_o r_o^2}{r_o^2 - r_i^2} \left(\frac{r^2 + r_i^2}{r^2}\right) \tag{102}$$

Where,

σ_θ = Hoop stress.

σ_r = Radial stress.

r_o = Outside radius.

r_i = Inside radius.

r = Radius at any point.

The radius at any point can be the outer or inner radius depending where the stress is estimated. This radius must be the outer radius when the stress is calculated at the outer surface.

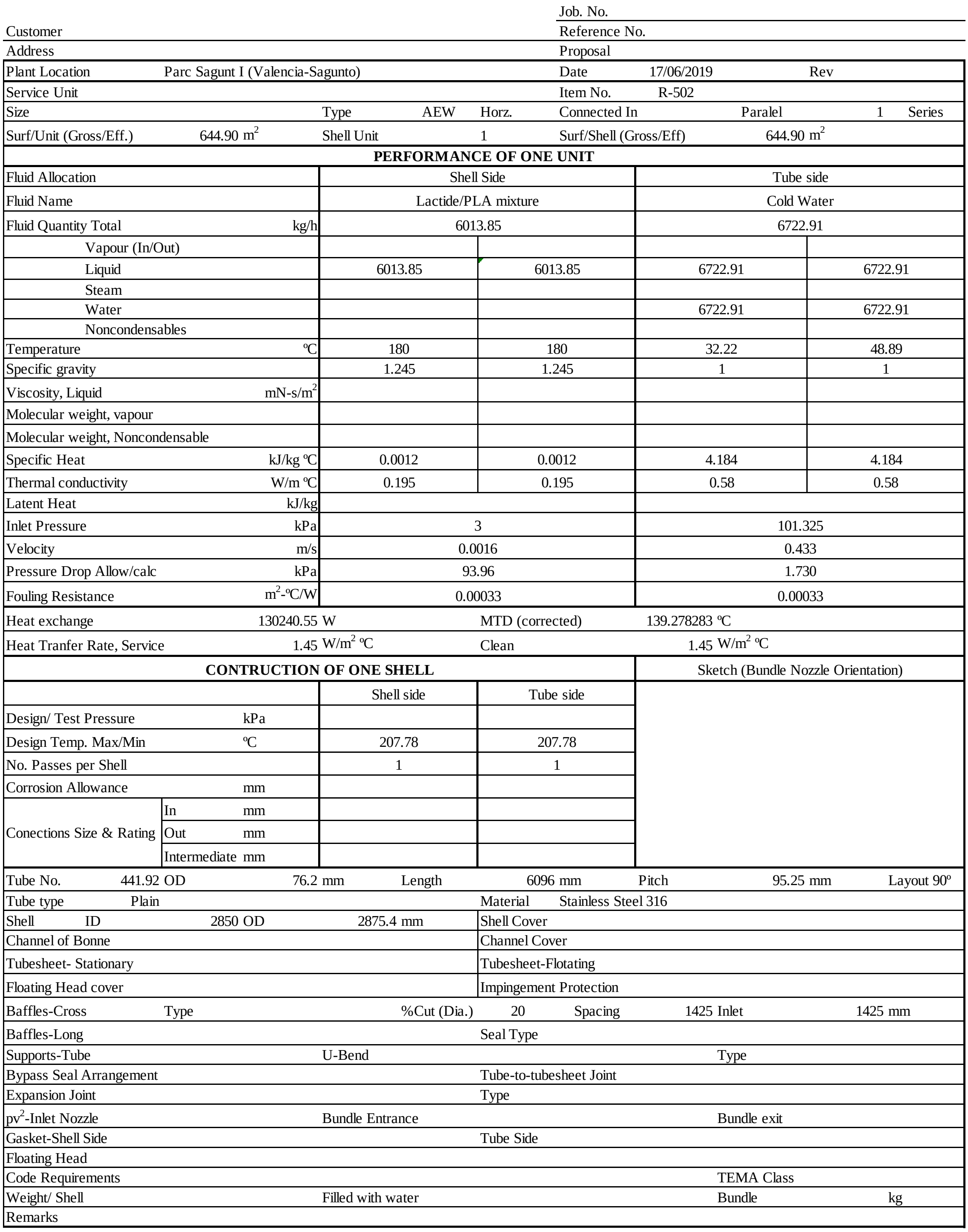
2.7 Final results

This section of the Annex II: Supporting Calculations includes all the results of the thermal and mechanical design of the reactor R-502, which has been design as a heat exchanger.

Most of the results can be collected in the specification sheet of the equipment, other results are gathered in normal tables. The figure 19 shown below is the specification sheet.

Table 8. Dimension of the reactor and different lengths for the shell. (Own authorship)

V (m^3)	19.94	**L_{ts} (mm)**	25.40
L_{bb} (mm)	26.25	**L_{tp} (mm)**	95.25
D_{octl} (m)	2.82	**$L_{tp,eff}$ (mm)**	95.25
D_{ctl} (m)	2.74	**L_{pp} (mm)**	95.25
L_{to} (m)	6.14	**L_{bc} (m)**	1.43



				Job. No.			
Customer				Reference No.			
Address				Proposal			
Plant Location	Parc Sagunt I (Valencia-Sagunto)			Date	17/06/2019	Rev	
Service Unit				Item No.	R-502		
Size		Type	AEW Horz.	Connected In	Paralel	1	Series
Surf/Unit (Gross/Eff.)	644.90 m^2	Shell Unit	1	Surf/Shell (Gross/Eff)	644.90 m^2		

PERFORMANCE OF ONE UNIT

Fluid Allocation		Shell Side		Tube side	
Fluid Name		Lactide/PLA mixture		Cold Water	
Fluid Quantity Total	kg/h	6013.85		6722.91	
Vapour (In/Out)					
Liquid		6013.85	6013.85	6722.91	6722.91
Steam					
Water				6722.91	6722.91
Noncondensables					
Temperature	ºC	180	180	32.22	48.89
Specific gravity		1.245	1.245	1	1
Viscosity, Liquid	mN-s/m^2				
Molecular weight, vapour					
Molecular weight, Noncondensable					
Specific Heat	kJ/kg ºC	0.0012	0.0012	4.184	4.184
Thermal conductivity	W/m ºC	0.195	0.195	0.58	0.58
Latent Heat	kJ/kg				
Inlet Pressure	kPa	3		101.325	
Velocity	m/s	0.0016		0.433	
Pressure Drop Allow/calc	kPa	93.96		1.730	
Fouling Resistance	m^2-ºC/W	0.00033		0.00033	
Heat exchange	130240.55 W	MTD (corrected)	139.278283 ºC		
Heat Tranfer Rate, Service	1.45 W/m^2 ºC	Clean	1.45 W/m^2 ºC		

CONTRUCTION OF ONE SHELL				Sketch (Bundle Nozzle Orientation)
		Shell side	Tube side	
Design/ Test Pressure	kPa			
Design Temp. Max/Min	ºC	207.78	207.78	
No. Passes per Shell		1	1	
Corrosion Allowance	mm			
Conections Size & Rating	In mm			
	Out mm			
	Intermediate mm			

Tube No.	441.92	OD 76.2 mm	Length 6096 mm	Pitch	95.25 mm	Layout 90º	
Tube type	Plain		Material	Stainless Steel 316			
Shell	ID 2850	OD 2875.4 mm	Shell Cover				
Channel of Bonne			Channel Cover				
Tubesheet- Stationary			Tubesheet-Flotating				
Floating Head cover			Impingement Protection				
Baffles-Cross	Type	%Cut (Dia.)	20	Spacing	1425 Inlet	1425 mm	
Baffles-Long			Seal Type				
Supports-Tube		U-Bend			Type		
Bypass Seal Arrangement			Tube-to-tubesheet Joint				
Expansion Joint			Type				
pv^2-Inlet Nozzle		Bundle Entrance			Bundle exit		
Gasket-Shell Side			Tube Side				
Floating Head							
Code Requirements					TEMA Class		
Weight/ Shell		Filled with water			Bundle	kg	
Remarks							

Figure 19. Specification sheet of the reactor R-502. Adapted from [11]

Table 9. Results of the calculations for the shell heat transfer coefficient. (Own authorship)

h_s (W/m^2 ºC)	1.500	**Re_s**	0.0002
h_i (W/m^2 ºC)	1.534	**G_s (kg/m^2-s)**	2.036
J_1	0.840	**D_w (m)**	0.16
J_c	1.081	**L_{bi} (m)**	1.62
J_b	0.968	**L_{bo} (m)**	1.62
J_s	1.674	**N_c**	95
J_r	0.665		

Table 10. Results of the calculation of the pressure drop in the shell (Own authorship).

P_s (kPa)	93.964	**R_b**	0.820
P_c (kPa)	1.291	**R_1**	0.035
P_w (kPa)	20.962	**R_s**	1.756
P_e (kPa)	71.711	**G_w (kg/m^2-s)**	2.298
$P_{b,i}$ (kPa)	20.029		

Table 11. Results of the heat transfer coefficient and pressure drop in the tubes (Own authorship).

h_t (W/m^2 ºC)	2167.106	**P_t (kPa)**	1.730
Re_t	58658.128	**j_f**	0.024
j_h	0.003	**A_t (m^2)**	0.004
G_t (kg/m^2-s)	433.136		

Table 12. Results of the calculations in the baffle window and the baffle. (Own authorship)

N_b	3	**F_w**	0.131
N_{tcc}	18	**F_c**	0.738
N_{tcw}	4	**θ_{ds} (rad)**	1.855
N_{tw}	58	**θ_{ctl} (rad)**	1.798

Table 13. Geometry of the equipment: Areas. (Own authorship).

S_m (m^2)	0.82	**S_b (m^2)**	0.092
S_{wg} (m^2)	0.91	**S_{sb} (m^2)**	0.046
S_{wt} (m^2)	0.26	**S_{tb} (m^2)**	0.037
S_w (m^2)	0.64		

Table 14. Results of the calculation of the overall heat transfer coefficient. (Own authorship)

R_{fo} (m^{2}°C/W)	0.0003	r_i (m)	0.037
R_{fi} (m^{2}°C/W)	0.0003	U (W/m^{2}°C)	1.450
t_w (m)	0.0021	k_w (W/m°C)	15.000
r_o (m)	0.0381		

Table 15. Results of the calculation of the shell thickness. (Own authorship)

$P_{external}$ (kPa)	101.325	E_0 (GPa)	200.000
$P_{allowable}$ (kPa)	153.115	D_0/t	226.409
A	0.0003	L/D_0	2.138
D_0 (m)	2.875	S_t (GPa)	0.017
t (mm)	12.700		

Table 16. Results of the calculation of stresses in the shell. (Own authorship)

	Inner surface	**Outer surface**
Radial stress (kN/m^{2})	0	11521.356
Hoop stress (kN/m^{2})	101.325	11420.031
Maximum deflection (m)	0.058	0.058

Table 17. Comparison of the allowable pressure in different heads. Selection of head and thickness. (Own authorship)

	Hemispherical head	**Ellipsoidal Head**	**Torispherical head**
D_i (mm)	2865.40	2865.40	2865.40
t (mm)	5.00	5.00	5.00
D_o (mm)	2875.40	2875.40	2875.40
R_o (mm)	1437.70	2587.86	2875.40
A	0.00043	0.00024	0.00022
B (MPa)	37.00	27.00	27.00
E (MPa)	193000.00	193000.00	193000.00
P_a (kPa)	128.68	52.17	46.95
h_o (mm)	-	716.35	-

3. Dimensions of other equipment

This section of the Annex II: supporting calculations includes some preliminary sizing of the equipment of the project and is not a complete design. The equipment to be design in this project is the reactor R-502, which includes both the thermal and the mechanical design.

3.1 Tanks

TK-101 is the initial storage tank for the raw material lactic acid, which is a liquid at atmospheric conditions. The volume of a tank can be sizing in agreement with equation 103.

$$V = Q\,\tau \tag{103}$$

Where,

V = Volume of the tank (m^3).

Q = Flow rate of the liquid leaving the tank (m^3/s)

τ = Residence time of the liquid stored in the tank (s).

An oversizing over 20% is required in order to fulfil the inherent safety conditions during design and operation. Once the volume of the tank has been estimated, standards dimensions of the tank must be considered. In fact, in table 7 are collected some standard dimensions for storage tanks.

Table 18. Storage tank standards. [16]

Diameter (m)	Height (m)	Capacity (m^3)
6.40	5.51	177.15
7.32	7.32	307.44
9.14	7.32	480.38
9.14	8.91	585.05
9.14	10.79	708.90
9.14	11.34	744.76
9.14	12.67	831.91
12.19	10.25	1196.51
15.24	14.55	2654.90
18.29	12.14	3189.21
21.34	12.22	4368.12
30.48	12.19	8896.00
45.72	14.63	24019.20

Table 19. Results of the sizing of tank TK-101. (Own authorship)

m (kg/h)	12970.71
Q (m^3/s)	0.0024
τ (d)	4
$V_{theoretical}$ (m^3)	813.10
$V_{oversizing}$ (m^3)	975.72
$V_{standardized}$ (m^3)	1196.9
H (m)	19.25
D (m)	12.19

The mixing vessel V-301 can also be dimensioning with equation 103 but the oversizing is going to be a 10% instead a 20%. The geometry of this mixing vessel is assumed cylindrical and can be estimated from the relationship between the height and diameter.

$$D_{tank} = \sqrt[3]{\frac{4\,V_{oversizing}}{\pi\left(\frac{H}{D_{tank}}\right)}} \qquad (104)$$

Where,

D_{tank} = Diameter of the tank (m).

H = Height of the tank (m).

Table 20. Results of the sizing of the stirrer storage tank V-301. (Own authorship)

Q (m^3/s)	0.0025
τ (min)	20
V (m^3)	3.05
$V_{oversizing}$ (m^3)	3.36
H/D	2
D (m)	1.24
H (m)	2.49

3.2 Pumps and pipelines

There are a total of 20 pumps in the poly (lactic acid) production facility. Many of them are common centrifugal pumps but there are also gear pumps for more viscous liquids (the polymer).

The total energy balance in a pump can be estimated in agreement with equation 105.

$$g\Delta z + \frac{\Delta P}{\rho} - \frac{\Delta P_f}{\rho} - W = 0 \qquad (105)$$

Where,

W = work to be done for the fluid to be pumped (J/kg).

Δz = Height difference (m).

ΔP = Pressure difference (Pa).

ΔP_f = Pressure losses due to friction in pipelines and equipment (Pa).

ρ = Density of the fluid to be pumped (kg/m^3).

g = Gravity acceleration (m/s^2).

The term of the velocity has not been included in the equation 105 because the suction and discharge pipelines are assumed to have the same diameter and the same velocity.

The power of the pump can be estimated once the work of the fluid is already known.

$$P = \frac{W\,Q\,\rho}{\eta} \qquad (106)$$

Where,

η = Efficiency of the pump.

The flow rate, the viscosity of the fluid, the density of the fluid, the pressure and the height in the points of reference for the application of the energy balance in the pump must be known.

The estimation of the characteristics of the pumps is preliminary for this project. The pipelines are not installed and for this reason the number of fittings and accessories are unknown. The real height of the equipment is also an unknown because not all the equipment has been design.

The calculation of the power of the pump has been estimated with the distance between equipment (in agreement with the layout in plant) and the losses through the pipelines.

The pressure drop in the pipelines is calculated in accordance with equation 107.

$$\Delta P_f = 8f\left(\frac{L}{d_i}\right)\frac{\rho u^2}{2} \qquad (107)$$

Where,

f = Friction factor.

L = Length of the pipeline (m).

d_i = Inside diameter of the pipeline (m).

u = Velocity of the fluid in the pipeline (m/s).

ρ = Density of the fluid (kg/m^3).

The friction factor can be obtained from a moody chart once the Reynolds number is known and the velocity can be calculated with equation 108.

$$v = \frac{Q}{\frac{\pi}{4} d_i^2} \tag{108}$$

Where,

Q = Flow rate (m^3/s)

The inside diameter of the pipeline can be estimated with two paths. The first path is an initial assumption. The diameter must be high enough in order to maintain the velocity of the fluid inside an expected normal range. The other paths is an economic estimation. As rule of thumb the equation 109 can be employed.

$$d_{i,optimum} = Q^{0.5} \tag{109}$$

Once the diameter is calculated must be standardized and the velocity of the fluid must be check.

Table 21. Results of the pumps calculations. (Own authorship)

	P-101 A/B	**P-102 A/B**	**P-201 A/B**	**P-301 A/B**	**P-302 A/B**	**P-502 A/B**
P (Pa)	0.00	28500.00	0.00	0.00	32500.00	0.00
Z (m)	0.00	0.00	0.00	0.00	0.00	0.00
W (J/kg)	40.69	115.81	40.33	62.77	39.49	65426.77
η	45%	45%	50%	80%	80%	80%
ρ (kg/m^3)	1179.60	1143.43	1233.46	1235.01	1250.00	1246.14
μ (kg/m·s)	0.01	0.00	0.00	0.00	0.00	1520.04
$L_{suction}$ (m)	5.00	5.00	5.00	7.21	13.45	5.00
$L_{discharge}$ (m)	5.00	5.00	5.00	13.00	8.94	5.66
P (W)	325.80	713.90	181.26	245.44	43.46	136620.35

Table 22. Results of the pumps calculations (continuation). (Own authorship)

	P-401 A/B	**P-402 A/B**	**P-403 A/B**	**P-404 A/B**	**P-405 A/B**	**P-501 A/B**
P (Pa)	0.00	0.00	0.00	0.00	28000.00	0.00
Z (m)	0.00	0.00	0.00	0.00	0.00	0.00
W (J/kg)	8.10	8.10	632.12	92.49	797.89	47958.57
η	45%	70%	45%	70%	45%	80%
ρ (kg/m^3)	29.11	31.44	1213.76	28.94	1231.32	1208.97
μ (kg/m·s)	0.00	0.00	0.00	0.00	0.00	61.84
$L_{suction}$ (m)	7.81	8.06	10.00	18.68	9.06	5.00
$L_{discharge}$ (m)	5.66	12.04	13.00	11.05	27.22	8.00
$L_{discharge}$ (m)	20.2485	70	-	65	-	-
P (W)	411.96	10755.59	2663.76	976.25	2958.09	100144.28

The results of the pipeline diameter are shown in Document II: Plans in the P&ID diagram.

3.3 Ejectors

The production process for the manufacturing of poly (lactic acid) has to be operated under vacuum conditions. The pressure below atmospheric level can be classified into rough, medium, high and ultra-high vacuum. The rough vacuum is the most used for industry and is ranged from atmospheric pressures to 1 torr (0.133 kPa). The lowest vacuum pressure for the facility explained in this project is 2 kPa, so a rough vacuum is also required.

The vacuum in the process is generated by vacuum equipment. Some of the most common are: steam ejectors, liquid ring pumps, rotary piston pumps, rotary vane pumps, rotary blowers, so as integrating pumping systems. [17]

The vacuum equipment chosen for this process are the steam jet ejector pumps or steam ejectors because they can handle corrosive vapours with good efficiencies. They have low costs, simple operation and stable operation. Moreover, they can have 3 micron (depending on the number of stages) as lowest suction pressure. A two-stage steam ejector can produce 1.6 kPa vacuum.

A jet pump is usually provided with 3 connections: motive medium inlet connection, suction manifold and pressure manifold. A mass balance can be applied for inlet and outlet in these connections.

$$\dot{M}_1 + \dot{M}_0 = \dot{M} \qquad (110)$$

Where,

M_1 = Mass flow rate in the suction manifold (kg/h).

$\dot{M}_0$ = Mass flow rate in the motive medium inlet connection (kg/h).

$\dot{M}$ = Mass flow rate in the pressure manifold (kg/h).

This project does not include a complete design of the steam ejectors used for vacuum requirements. However, a preliminary analysis of the steam consumption in the ejector is explained.

The consumption of steam in ejectors depends on the compression ratio, the expansion ratio, the composition of the suction flow, the mean molecular weight and the temperatures.

$$E = \frac{P_1}{P_0} \qquad (111)$$

Where,

E = Expansion ratio.

P_1 = Motive stream pressure.

P_0 = Suction pressure.

$$K = \frac{P}{P_0} \tag{112}$$

Where,

K = Compression ratio.

P = Discharge pressure.

Both parameters have a strong relationship because the smaller and the higher the values of K and E respectively, a lesser consumption of steam is required.

The steam consumption of the ejectors can be estimated in agreement with equation 113.

$$\dot{M}_1 = \dot{M}_{owe}\ b \tag{113}$$

Where,

M_{owe} = Equivalent water vapour suction flow (kg/h).

b = Parameter from figure 20.

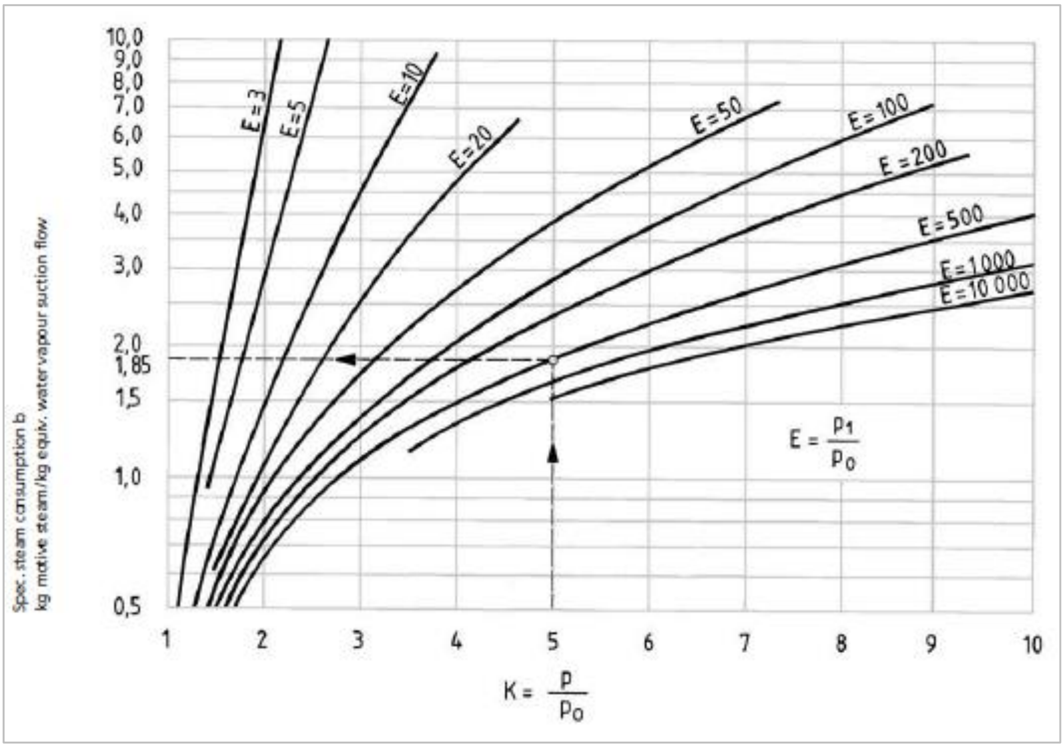


Figure 20. Steam consumption per equivalent water vapour suction flows. [18]

The equivalent water vapour suction flow can be calculated with equation 114.

$$\dot{M_{02}} = \dot{M_{01}} \frac{f_2}{f_1} \tag{114}$$

Where,

M_{01} = Actual suction flow (kg/h).

f_2 = Equivalent suction flow factor.

f_1 = Suction flow factor.

The total equivalent water vapour suction can be calculated from the total amount of water in the suction and the amount of other vapour mixtures converted to equivalent water.

$$\dot{M_{02T}} = \dot{M_{02}}' + \dot{M_{02}}'' \tag{115}$$

Where,

$\dot{M_{02}}'$ = Flow rate of water or water vapour (kg/h).

$\dot{M_{02}}''$ = Flow rate of equivalent water of other vapour mixtures (kg/h).

The suction factor and equivalent suction factor are estimated from figure 21, where the inlets are the suction temperature, the motive stream temperature and the average molecular weights of the water and the vapour mixture.

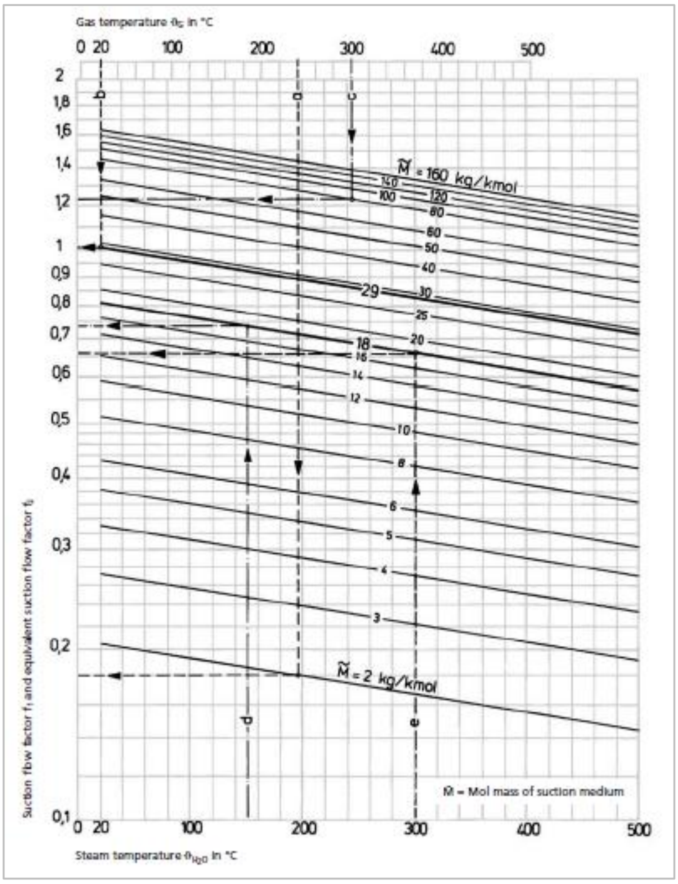


Figure 21. Suction and equivalent suction factors. [18]

The final results for the steam jet ejectors required in the production facility of poly (lactic acid) are shown in tables 8 and 9.

Table 23. Results for the consumption of steam in ejectors.

	EJ-101	EJ-201	EJ-202	EJ-301	EJ-401
P_1 (kPa)	4136.85	4136.85	4136.85	4136.85	4136.85
P_0 (kPa)	6.50	35.00	50.00	2.50	2.00
P (kPa)	50.00	50.00	101.33	6.00	15.00
E	636.44	118.20	82.74	1654.74	2068.43
K	7.69	1.43	2.03	2.40	7.50
b	3.00	0.5	0.92	1.00	2.20
M_1 (kg/h)	7383.36	843.15	2797.90	3765.56	640.54
M_{owe} (kg/h)	2461.12	1686.30	3041.20	3765.56	291.16

Table 24. Results for the consumption of steam in ejectors (continued).

	EJ-402	EJ-403	EJ-404	EJ-405	EJ-406	EJ-601
P_1 (kPa)	4136.85	4136.85	4136.85	4136.85	4136.85	4136.85
P_0 (kPa)	15.00	2.00	15.00	2.00	15.00	6.500
P (kPa)	101.33	15.00	101.33	15.00	101.32	30.000
E	275.79	2068.43	275.79	2068.43	275.79	636.44
K	6.76	7.50	6.76	7.50	6.75	4.62
b	3.50	2.20	3.50	2.2	3.50	1.75
M_1 (kg/h)	599.05	36.57	22.32	1341.28	4180.01	242.31
M_{owe} (kg/h)	16.62	16.62	6.38	609.67	1194.29	138.46

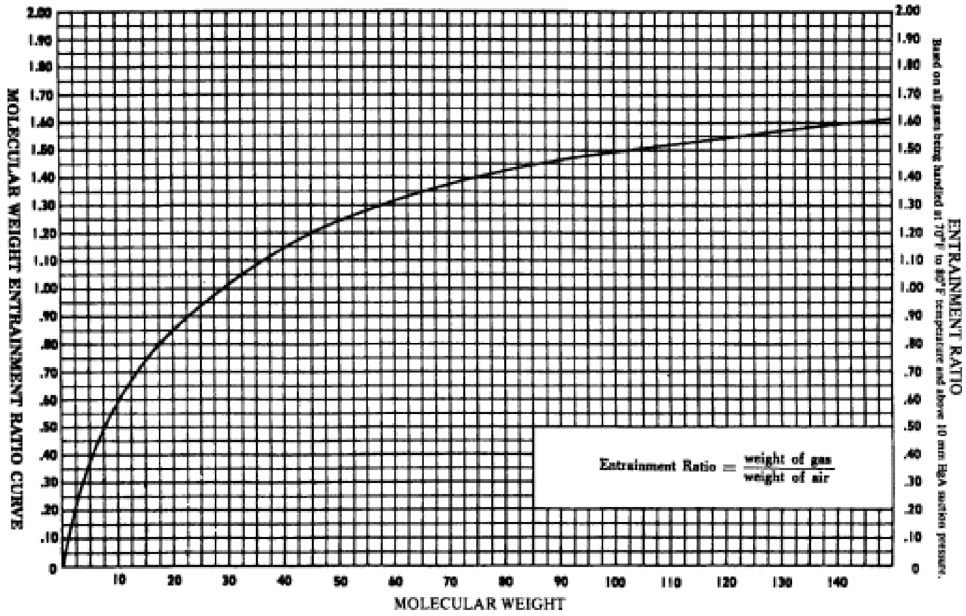


Figure 22. Molecular weight entrainment ratio. [17]

The air equivalent of the mass flow rate mixture in the suction manifold can be estimated from the entrainment ratio. This ratio has a relationship with the mean average molecular weight in accordance with figure 22. Once the entrainment ratio is known, the total mass flow rate in the suction manifold is divides by this parameter and the air equivalent is finally known.

3.4 Heat exchangers

Heat exchangers, reboilers and condensers are included in this section of the Annex II: Supporting calculations. This project has a total of 15 heat transfer equipment without including any main equipment. The named equipment is: E-102, E-103, E-301, E-302, E-401, E-402, E-403, E-404, E-405, E-406, E-407, E-408, E-409, E-410, E-601.

The complete design of a heat exchanger includes the thermal and mechanical design which is a very long procedure. Some of the previously mentioned heat exchangers have a shell and tube configuration and can be design in agreement with the procedure indicated for reactor R-502.

Because of the dimensions of this production facility, a very preliminary sizing of the heat exchangers is shown. The main parameters to consider for this sizing are: process temperature inlet and outlet, utility temperature inlet and outlet, the heat load and heat transfer area.

The calculation of the heat transfer area was made taking into account equation 31. The overall heat transfer coefficient is going to be assumed, otherwise a complete thermal design is required.

The process fluid is generally in the tube side of the heat exchangers because of the corrosive properties of the lactic acid and the low vacuum, except in process streams with a higher viscosity just like stream 21.

The heat transfer overall coefficient has been chosen with the information in table 10.

Table 25. Values of the overall heat transfer coefficient. [13]

Service fluid	**Process fluid**	**U (W/m^2°C)**
Water	Vacuum condenser	200-500
Steam	Aqueous solutions	1000-1500
Steam	Heavy oils	60-450
Water	Aqueous vapours	1000-1500

Some of the overall transfer coefficients were taken from figure 23.

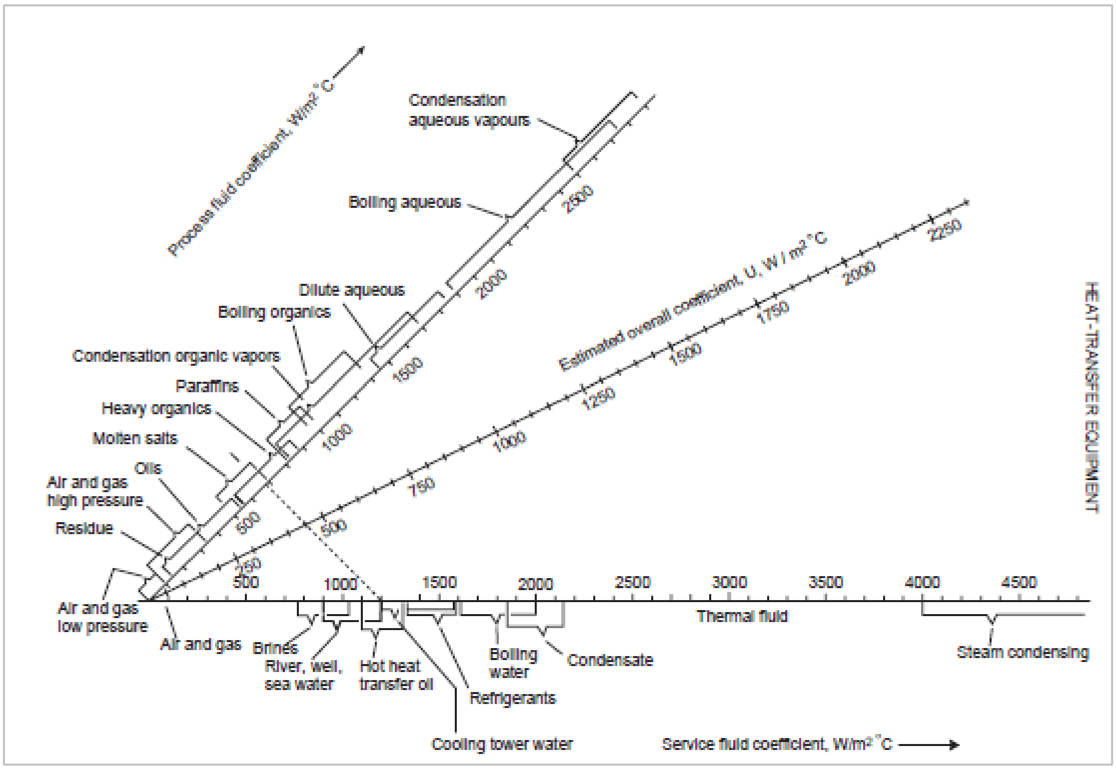


Figure 23. Overall heat transfer coefficients. [13]

The results of the preliminary sizing of the heat exchangers is shown in table 25.

Table 26. Sizing of the heat exchangers. (Own authorship)

	A (m^2)	U (W/m^2 ºC)	LMTD (ºC)
E-102	17.70	200	96.89
E-103	10.07	1000	37.49
E-301	12.28	100	57.18
E-302	30.34	500	116.72
E-401	11.08	300	87.22
E-402	27.11	1000	13.67
E-403	2.16	200	113.50
E-404	20.42	300	87.22
E-405	51.20	1000	12.07
E-406	0.35	100	110.83
E-407	13.12	200	92.17
E-408	1.63	600	86.04
E-409	2.13	1000	59.83
E-410	9.74	700	23.85
E-601	4604.80	60	36.41

All the heat exchangers with an area lower than 10 m^2, except E-410, are double pipe exchangers.

3.5 Distillation columns

This section introduces a preliminary sizing of columns T-401, T-402 and T-403. This sizing will includes the diameter, the length, the thickness and the mass of the column without accessories. The last parameter is important for the Document IV: Budget.

The first step in the determination of the diameter of the column is to determine the correlation given by equation 116.

$$X = \frac{L}{G}\left(\frac{\rho_g}{\rho_l}\right)^{0.5} \tag{116}$$

Where,

X = Flow parameter.

L = Liquid mass flow (kg/h).

V = Vapour mass flow (kg/h).

ρ_g = Density of the gas (kg/m^3).

ρ_l = Density of the liquid (kg/m^3).

From the flow parameter and with figure 24 the modified flooding parameter can be determined.

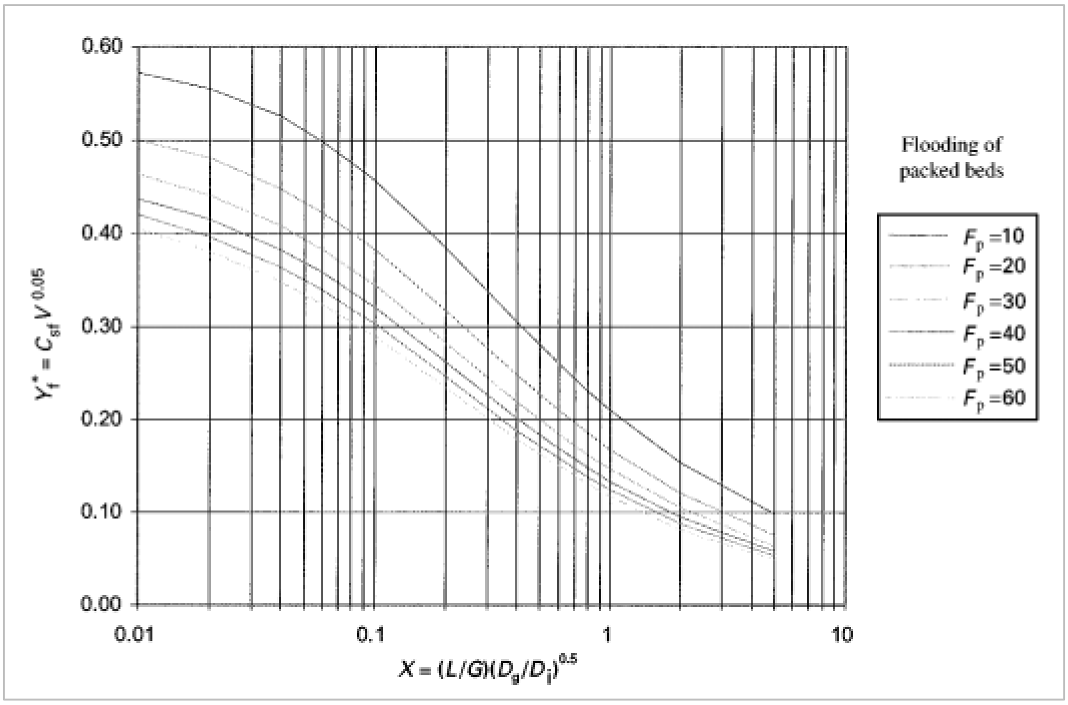


Figure 24. Modified flooding parameter curve as function of the flow parameter. [19]

The packing factor required for figure 24 depends on the type of the packing selected for the column. The structured packing provided by Sulzer with a size of 125 Y has a packing factor with a value of 10.

The modified flooding parameter is expressed as,

$$Y_f^* = C_s \gamma^{0.05} \tag{117}$$

Where,

C_s = Vapour capacity factor (m/s)

γ = Kinematic viscosity constant.

The kinematic viscosity constant is calculated with equation 118.

$$\gamma = \frac{\mu_l}{S_g} \tag{118}$$

Where,

μ_l = Liquid viscosity (kg/m·s)

S_g = Liquid specific gravity.

The vapour velocity is estimated with the equation 119.

$$u_g = C_s \frac{(\rho_l - \rho_g)^{0.5}}{\rho_g} \tag{119}$$

The flooding gas mass velocity can be obtained from the vapour velocity

$$G_{fl} = \frac{u_g}{\rho_g} \tag{120}$$

The column cross sectional for an 80% flooding is determined with equation.

$$A_c = \frac{V}{(0.8\, G_{fl})} \tag{121}$$

Where,

V= Vapour flow (kg/h)

Finally the column diameter is obtained from equation 122.

$$D_c = \left(\frac{4A_c}{\pi}\right)^{0.5} \tag{122}$$

The results data and results from the calculation of the diameter of the column T-401, T-402 and T-403 is provided in table 27.

Table 27. Results of the diameter of the column. (Own authorship)

	T-401	**T-402**	**T-403**
L (kg/h)	2358.82	3641.65	492.43
G (kg/h)	6190.23	4097.21	1313.14
X	0.02	0.05	0.02
ρ_g (kg/m^3)	0.08	0.09	0.08
ρ_l (kg/m^3)	29.11	31.44	28.94
F_p	10	10	10
Y_f*	0.58	0.53	0.58
γ (kg/m·s)	0.097	0.089	0.091
μ_l (kg/m·s)	0.0028	0.0028	0.0026
S_g	0.029	0.031	0.029
C_s	0.65	0.60	0.65
u_g (m/s)	43.68	39.12	42.19
G_{fl} (kg/m^2·s)	543.21	457.01	506.91
V (kg/h)	6190.23	3896.47	1313.14
A_c (m2)	14.24	10.66	3.24
D_c (m)	4.26	3.68	2.03
L (m)	21.29	18.42	10.15

According to heuristics a column must have a height between 2-50 m and a diameter between 0.03- 4 m. Moreover, the ratio between the height and the length must be in a range 2-30. An approximate ratio of 5 has been chosen as estimation and the final results are collected in table 27.

The thickness of the column is calculated by following the procedure explained in section 2.6.6 of this annex. The results from this calculations are shown in table 28.

Table 28. Thickness and mass of the column T-401, T-402 and T-403. (Own authorship)

	T-401	**T-402**	**T-403**
t (mm)	25.40	19.05	12.70
E (Mpa)	179000	179000	179000
D_0/t	165.17	190.18	157.59
L/D_0	4.94	4.95	4.94
A	0.0001	0.0001	0.00017
B (MPa)	16	16	17
P (kPa)	129.16	112.18	143.83
Mass (kg)	54754.86	30725.03	6223.54

The factor B is ouside the elactic region for the thickness calculation of the columns. The allowable pressure must be calculated, then, with equation 123.

$$P_a = \frac{4\,B}{3\left(\frac{D_o}{t}\right)} \tag{123}$$

The mass of the shell of the column can be calculated with equation 124.

$$Mass_{column} = \pi d_i L\,t\,\rho \tag{124}$$

The inside diameter, the thickness and the length must be expressed in m in the equation 124. The density of the column material is 7990 kg/m^3 (stainless steel 316).

3.6 Vessels

V-101, V-401, V-402, V-403, V-404, V-601 are going to be sized in this section as phase-separators. The preliminary design can be made taking into account heuristics.

The first step for this design is the calculation of the gas velocity.

$$v_g = k\sqrt{\frac{\rho_l}{\rho_g} - 1}\; m/s \tag{125}$$

Where,

ρ_l = Density of the liquid (kg/m^3).

ρ_g = Density of the gas (kg/m^3).

k = Constant value of 0.0305 for vessels without mesh entrainment and 0.11 for vessels with mesh entrainment. [20]

A popular efficiency of these type of equipment is a 75% of the gas velocity.

The volume of the liquid in the vessel can be estimated with equation 126.

$$V_{liquid} = \frac{LF\,\frac{\tau}{60}}{\rho_l} \tag{126}$$

Where,

LF = Liquid flow rate (kg/h).

τ = Hold up time (min).

The diameter of the vessel can be estimated with equation 127.

$$D_v = \sqrt{\frac{VF\ 4}{v_g \rho_g \pi}} \tag{127}$$

Where,

VF = Vapor flow rate (kg/h).

The length of the separator is obtained from equation 128. The dimensions of the vessel were determined for a half full equipment.

$$L_v = \frac{8}{\pi {D_v}^2} \tag{128}$$

The results of the table 29 were obtained with the equations explained before.

Table 29. Results of the phase-separator dimensions. (Own authorship)

	V-101	**V-401**	**V-402**	**V-403**	**V-404**	**V-601**	**V-405**
Type of vessel	Vertical	Vertical	Vertical	Vertical	Vertical	Vertical	Horizontal
v_g (m/s)	0.465	1.094	2.070	0.880	2.812	2.127	-
k	0.110	0.031	0.110	0.031	0.031	0.031	-
ρ_l (kg/m^3)	6.194	29.111	37.940	92.863	1210.920	1250.000	1231.32
ρ_l (kg/m^3)	0.329	0.023	0.107	0.111	0.142	0.257	-
FV (kg/h)	2027.036	456.806	248.661	34.520	7.957	305.955	-
FL (kg/h)	957.140	6290.179	208.145	4248.588	26.563	5708.393	15.16
v_g (75% efficiency)	0.349	0.821	1.553	0.660	2.109	1.595	-
τ (min)	10.000	5.000	5.000	0.200	5.000	5.000	10.000
V_{liquid} (m^3)	25.754	18.006	0.457	0.153	0.002	0.381	0.002
D_v (m)	2.502	2.952	0.728	0.407	0.097	0.514	0.300
L_v (m)	10.479	5.263	2.195	2.340	0.497	3.672	0.058
L_v/D_v	4.189	1.783	3.015	5.743	5.134	7.147	0.194

For vertical vapour-phase separators the ratio between the length of the equipment and the diameter is in a range of 2.5-5. The range of the height must be between 2-10 m and the diameter must be in a range of 0.3-2 m according to heuristics. V-401, V-404, V-405 and V-601 does not fulfilled the heuristics. For this reason, their dimensions were recalculated.

Table 30. Results of the recalculations. (Own authorship)

	V-401	**V-404**	**V-601**	**V-405**
Diameter of the vessel (m)	2	0.3	0.734	0.3
Length of the vessel (m)	10	2	3.672	2

The thickness and the mass of the phase-separators or drums can be estimated with the same procedure used for the columns. The thickness is calculated for a full vacuum pressure design.

Table 31. Results of the calculation of thickness and mass of the shell. (Own authorship)

	V-101	**V-401**	**V-402**	**V-403**	**V-404**	**V-405**	**V-601**
t (mm)	12.70	12.70	4.45	3.18	2.54	2.54	4.45
E (Mpa)	179000	179000	179000	173.931342	179000	179000	179000
D0/t	198.987	159.480	165.83	130.32	120.11	120.110	167.207
L/D0	4.146	4.937	2.98	5.65	6.56	6.556	4.940
A	0.00013	0.00015	0.00025	0.00018	0.0001	0.0001	0.00018
B (MPa)	17	13	24	17	16	16	17
P (kPa)	113.91	108.69	192.97	173.93	177.61	177.61	135.56
Mass (kg)	8356.97	6375.74	178.37	75.97	38.25	38.25	300.84

3.7 Evaporator and Reactors

There are 4 reactors and 1 main evaporator in these project. The reactor R-502 has already been sized and design. This section will included some dimensioning of the other 3 reactors and the evaporator.

Except for reactor R-501, the equipment can be sized as heat exchangers and the procedure to be followed is the same as the one indicated in the section 3.4 of this annex.

Reactor R-501 is sized with the same procedure that V-301.

The nomenclature in tables 32 and 33 is the same of the equation 30.

Table 32. Results of the sizing of reactor R-201. (Own authorship)

Q (kW)	74176.90
$T_{h,i}$ (ºC)	180
$T_{h,o}$ (ºC)	180
$T_{c,i}$ (ºC)	32.22
$T_{c,o}$ (ºC)	152.34
LMTD (ºC)	71.69
F	1
U ($W/m^{2o}C$)	350
A_o (m^2)	2.96

Table 33. Results of the sizing of reactor R-301. (Own authorship)

Q (kW)	155.11
$T_{h,i}$ (ºC)	252.33
$T_{h,o}$ (ºC)	252.33
$T_{c,i}$ (ºC)	220.00
$T_{c,o}$ (ºC)	220.00
LMTD (ºC)	32.33
F	1
U ($W/m^{2o}C$)	600
A_o (m^2)	0.008

Table 34. Results of the sizing of reactor R-301. (Own authorship)

Q (m^3/s)	0.0014
τ (min)	30
V(m^3)	2.561
$V_{oversizing}$ (m^3)	2.82
H/D	3
D (m)	1.03
H (m)	3.08

3.8 Relief valve

A vacuum relief valve can be defined as a pressure relief valve which is installed to admit fluid and prevent excessive internal vacuum. The valve recloses after the normal conditions are restored.

The main purpose of the relief sizing is to determine the discharge area of the valve and the diameter of the inlet and outlet piping. Vessels operating under partial vacuum have relief valves which can be design as pressure relief valves. Although API Recommended Practice 520 have explanations for the sizing of pressure valves, the methodology can also be applied to vacuum valves. For this specific case the pressure for the design is going to be a gauge pressure and new terms like maximum allowable working vacuum (MAWV) can be defined. The higher pressure is in the outside part of the vessel (reactor R-201). The sizing will be made, then, considering as maximum allowable working pressure the design pressure which is the difference between the vacuum pressure and the atmospheric pressure.

The sizing of a relief valve is different depending on the fluid released from the system, or introduced. Valve VSV-202 was designed taking into account that a gas (nitrogen) is introduced in the reactor to reduce the vacuum. The design would be also different depending of the type of flow: critical and subcritical. Therefore, the first step is the calculation of the critical or subcritical conditions. Equation 129 is the expression for the critical flow ratio calculation.

$$\frac{P_{cf}}{P_1} = \left[\frac{2}{\gamma + 1}\right]^{\gamma} \tag{129}$$

Where,

P_{cf} = Critical flow pressure in the nozzle (kPa).

P_1 = Pressure of the relief (kPa).

γ = Ratio of specific heats (C_p/C_v).

The final results for the critical flow calculation are shown in table 35. All of these results are referred to atmospheric pressure.

Table 35. Results and input data for the critical flow calculation.

Design pressure for the Reactor (kPaa)	101.325
Maximum allowable vacuum pressure (kPaa)	101.325
Valve set pressure (kPaa)	91.193
Allowable overpressure (%)	10
Back pressure (kPaa)	0
Relieving pressure, P_1 (kPaa)	91.284
Critical flow pressure, P_{cf} (kPaa)	106.508

As the critical flow pressure is higher than the downstream pressure, the discharge area of the relief valve can be estimated as critical flow with equation 130.

$$A = \frac{13160\, W}{C\, K_d P_1 K_b K_c}\sqrt{\frac{TZ}{M}} \tag{130}$$

Where,

W = Flow rate through the relief valve (kg/h).

C = Coefficient from equation 115.

K_d = Effective coefficient of discharge.

K_b = Correction factor for backpressure.

K_c = Correction factor for combined systems with rupture discs.

T = Temperature of the inlet gas (K).

Z = Compressibility factor due to deviations from ideal behaviour of gases.

M = Molecular weight of the gas (kg/kmol).

$$C = 520\sqrt{\gamma\left[\frac{2}{\gamma+1}\right]^{(\gamma+1)/(\gamma-1)}} \tag{131}$$

The effective coefficient of discharge is assumed to be 0.975 for installed relief valves, the correction factor for backpressure is equal to 1 and the correction factor for combined systems is 1 because there is not rupture discs installed.

The flow rate through the relief valve must be estimated equal to the vapour stream of the reactor R-201 because the ejector originates the vacuum with the removal of the vapour of this stream.

The results and information required for the discharge area estimation are shown in table 36.

Table 36. Discharge area for relief valve VSV-202.

W (kg/h)	1895.958
K_c	1
K_d	0.975
C	356.060
K_b	1
T (ºC)	20
Z	1
M (kg/kmol)	28
$A_{calculated}$ (mm^2)	1153
$A_{standar}$ (mm^2)	1186

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ANNEX III

Economic viability analysis

Index

1. Introduction

The evaluation of any project, like the one explained on this document, requires an economic analysis in order to determine its feasibility and to ensure that the project can be undertaken. Future benefits are expected and the net earnings must be greater than the capital costs. This is a abrupt definition of a profitable project. The profitability can be assessed with methods like: payback period, return on investment, net present value, net return rate, capitalized cost, present value ratio and equivalent maximum investment, among others. Some of them are calculated in this economic analysis to determine the viability of this project.

2. Project characteristics

2.1 Initial funding

The materialization of a project cannot be possible without economical support. There are different ways to obtain the required funding of the project. Some of the most common are loan or credits of financing entities, public funding or own capital, although there are others like ‘crowdfunding’ or ‘bartering’. This project is going to be completely funded by external capital (a loan). More particularly, this project is funded by the ICO line (“Instituto de Crédito Oficial”) because the annual percentage rate is lower than other entities. The loan would be returned in fractions with constant rates. [1]

The repayment of the loan is made in fractions per year in such way that at the end of the payment period the loan is redeemed. Each year will be paid a constant quote in agreement with equation 1. [2]

$$A = P\,\frac{[i\,(1+i)^n]}{[(1+i)^n - 1]} \tag{1}$$

Where,

A= Annual payment (€).

P = Amount of money invested and required in the loan (€).

i = Annual percentage rate (%).

n = Life of the loan (years).

The accumulated loan can be estimated as a subtraction of the left amount required for repayment for each year and the loan payment of the actual one.

$$Accumulated\ loan = Accumulated\ loan_{n-1} - loan\ payment_n \tag{2}$$

The loan payment is difference between the annual payment and annual interest.

$$Loan\ payment = A - I \tag{3}$$

Where, the annual interest can estimated as the accumulated loan of the previous year multiply by the annual percentage rate.

The results of the funding considerations with agreement to equations 1, 2 and 3 are introduced in tables 6, 7, 8, 9 and 10 with the cash flow results.

Such calculations were performed taking into account the initial information provided in table 1.

Table 1. Loan information for calculations.

Loan required (€)	126,054,228.36 €
Average life of the project (year)	15.00
Annual Percentage Rate (APR)	5.09%

2.2 Revenues

An annual revenue is a constant value which specifies the amount of money received during one year of the plant production, which is the income obtained from the sales of the products and by-products. These project has only one product (polylactic acid) and the profits will be obtained from its sales. The revenues will be calculated from the addition of the volume of production with the price of the product in €/tonne.

Table 2. Revenues of the polylactic acid facility.

REVENUES	
Item	**Benefit (€/year)**
1. Polylactic acid	262,986,912.55 €
TOTAL	262,986,912.55 €

2.3 Manufacturing costs

2.3.1 Variable costs of production

The variable costs depends on the production activity of the facility. Some of the most relevant are the waste treatment, the raw materials cost, the consumables cost (like catalyst and stabilizers) and the utilities cost. The costs were calculated with its respective price per ton and its amount in ton per year. The results are shown in table 3.

Table 3. Results of the variable costs of production. (Own authorship)

VARIABLE OPERATING COSTS	
Item	**Cost (€)**
1. Raw materials	145,296,777.42 €
2. Utilities	5,727,484.51 €
3. Consumables	4,150,671.35 €
4. Waste treatment	1,730.67 €
TOTAL	155,176,663.95 €

2.3.2 Fixed costs of production

The costs of production remains invariable, regardless the rate of the industrial activity of the facility. The labor costs, maintenance, supervision and insurances, among others, are included between these types of costs.

The labor costs are mainly the salaries of the operators working in the plant. The salary of each operator is different and will depend on its function (maintenance, operation, services, commercial, investigation…), its responsibility, its experience, its knowledge and other similar criterion. In fact, the minimum salaries for the chemical industry are compiled in the resolution 26 of July of 2018, of the General Direction of the Work, in which is recorded and published the collective agreement of the general chemical industry. The minimum salaries are categorized into 8 groups, which depend of the level of formation and responsibility of the job post of the worker being group 8 the highest level. However, and being aware of the diversity of job post, an average salary will be considered. The salaries of the workers is 38,336 €. [3]

This facility operates with a shift-work basis with four shifts and an average of 4.8 workers per shift, which gives a total of approximately 20 workers.

Table 4 provides the results of some the most significant fixed costs.

Table 4. Fixed operating costs results. (Own authorship)

FIXED OPERATING COSTS	
Item	**Cost (€)**
1. Labour costs	736,051.20 €
2. Supervision	184,012.80 €
3. Maintenance	1,711,923.15 €
4. General Overhead expense	1,591,183.33 €
5. Direct Salary overhead	414,028.80 €
TOTAL	4,637,199.27 €

The supervision is considered the 25% of the operating labor, the direct salary overhead the 45% of the labor and supervision, the maintenance de 3% of the investment of the battery (equipment, piping, control…) of the facilities and the general overhead expense is the 65% of the labor and maintenance. [2]

2.4 Project life

The project life is the considered time to perform an economic analysis and other prospective estimations for the determination of the viability of the project. In chemical industry, a project life period between 10 and 20 years is expected. Analysis without these range is not recommended due to the volatility of the current global market.

The polylactic acid facility described in this project will considered a project life of 15 years to perform the economic analysis.

2.5 Annual repayments, amortization

The corporation tax document ("Impuesto sobre Sociedades") updated in the 10 January of 2019 and uploaded by the "Boletín Oficial del Estado" compiles some of the most important legislation regarding taxes to enterprises.

The law 27/2014 of November about the corporation taxes includes on its article 12 the maximum period of time for the amortization of material investments. Some relevant data are provided for the equipment and the industrial buildings, which maximum period of time for amortization is 18 and 68 years, respectively. These periods are not restrictive because are higher than the project life time. The annual amortization is assumed constant and can be estimated in agreement with equation 4.

$$Annual\ amortization = \frac{Amortizable\ material\ (€) - Residual\ value\ of\ materials\ (€)}{Useful\ life\ (years)} \tag{4}$$

The total amount of amortizable materials is shown in table 5 and the final result of the annual amortization is introduced in tables 6, 7, 8, 9 and 10.

Table 5. Amount of amortizable materials (€). (Own authorship)

AMORTIZATION/REPAYMENT	
Item	**Cost (€)**
1.Total of equipment	22,825,641.96 €
2.Total of off-sites	4,565,128.39 €
3.Total of instrumentation and control	4,565,128.39 €
4.Total of equipment erection	9,130,256.79 €
5.Total of piping	15,977,949.37 €
6.Total of utilities	11,412,820.98 €
TOTAL	68,476,925.89 €

3. Cash flows

3.1 Introduction

The cash flows are economic factors when determining a decision over the capital investment. They are calculated from the revenues and expenses, where the revenues are the cash inflows and the expenses the cash outflows. The cash flows can be estimated, then, as the profits after taxes subtracted by the loan payment. The profits after taxes include expenses related to variable costs of operation, fixed costs of operation, annual repayments (amortization) and corporation taxes imposed by the government. [4] There are also important the discounted cash flows and the accumulated cash flows. The first one established a relationship with the money in the future.

$$CF_{discounted} = \frac{CF}{(1+i)^n} \tag{5}$$

The accumulated cash flows can be estimated as,

$$CF_{accumulated} = -P + \sum_{n=0}^{n} CF_{discounted} \tag{6}$$

3.2 Rate of inflation and taxes

The rate of inflation is a percentage coefficient which highlights the increase of prices in a period of time. The current average inflation rate for Spain in 2019 is of 1.15%. [5]

The law 27/2014 includes, on its article 29 the type of taxes for economic activities. Entities of new creation will have a type of 15% taxes in the first year of operation, while the normal tax percent is 25%. According to these information, the described project will have a 15% taxes in the first year and 25% taxes the rest of the years.

3.3 Interest rate

The value of the money with time can be determine with the discounting rate, which is necessary when calculating the discounted cash flows. The discounting rate can be defined differently for external and own funding resources and for each case is called "cost of the debt" and "cost of opportunity", respectively. The discounting rate can be defined as,

$$Discountin\ rate = minimum\ required\ return + risk\ differential \tag{7}$$

Where, the risk differential is not considered for this project due to low uncertainly. The minimum required return is the cost of the resources, which is the cost of the debt in this project because of the type of funding. The discounting rate is then equal to the annual percentage rate of the loan.

3.4 Cash flow results

Table 6. Cash flow and other results. (Own authorship)

Year	**0**	**1**	**2**
Revenues (Incomes)	0.00 €	262,986,912.55 €	266,011,262.04 €
Fixed cost of production	0.00 €	-4,637,199.27 €	-4,690,527.06 €
Variable costs of production	0.00 €	-155,176,663.95 €	-156,961,195.59 €
Annual repayment	0.00 €	-4,565,128.39 €	-4,565,128.39 €
Profits before taxes	0.00 €	98,607,920.93 €	99,794,410.99 €
Taxes	0.00 €	14,791,188.14 €	24,948,602.75 €
Profits after taxes	0.00 €	83,816,732.79 €	74,845,808.25 €
Interest of the loan	0.00 €	6,472,849.61 €	6,174,931.55 €
Loan payment	0.00 €	5,851,857.40 €	6,149,775.46 €
Accumulated loan payment	127,142,989.80 €	121,291,132.40 €	115,141,356.94 €
Cash Flow	-127,142,989.80 €	77,964,875.39 €	68,696,032.78 €
Discounted cash flow	-127,142,989.80 €	74,187,966.04 €	62,201,464.20 €
Accumulated Cash Flow	-127,142,989.80 €	-52,955,023.77 €	9,246,440.43 €

Table 7. Cash flow and other results (continuation). (Own authorship)

	3	**4**	**5**
Revenues (Incomes)	269,070,391.55 €	272,164,701.06 €	275,294,595.12 €
Fixed cost of production	-4,744,468.13 €	-4,799,029.51 €	-4,854,218.35 €
Variable costs of production	-158,766,249.34 €	-160,592,061.20 €	-162,438,869.91 €
Annual repayment	-4,565,128.39 €	-4,565,128.39 €	-4,565,128.39 €
Profits before taxes	100,994,545.70 €	102,208,481.95 €	103,436,378.47 €
Taxes	25,248,636.42 €	25,552,120.49 €	25,859,094.62 €
Profits after taxes	75,745,909.27 €	76,656,361.46 €	77,577,283.85 €
Interest of the loan	5,861,846.48 €	5,532,822.25 €	5,187,047.40 €
Loan payment	6,462,860.53 €	6,791,884.76 €	7,137,659.61 €
Accumulated loan payment	108,678,496.41 €	101,886,611.65 €	94,748,952.04 €
Cash Flow	69,283,048.74 €	69,864,476.70 €	70,439,624.24 €
Discounted cash flow	59,693,963.59 €	57,278,852.91 €	54,952,747.06 €
Accumulated Cash Flow	68,940,404.02 €	126,219,256.93 €	181,172,003.99 €

Table 8. Cash flow and other results (continuation). (Own authorship)

Year	**6**	**7**	**8**
Revenues (Incomes)	278,460,482.96 €	281,662,778.52 €	284,901,900.47 €
Fixed cost of production	-4,910,041.86 €	-4,966,507.34 €	-5,023,622.18 €
Variable costs of production	-164,306,916.91 €	-166,196,446.46 €	-168,107,705.59 €
Annual repayment	-4,565,128.39 €	-4,565,128.39 €	-4,565,128.39 €
Profits before taxes	104,678,395.80 €	105,934,696.33 €	107,205,444.31 €
Taxes	26,169,598.95 €	26,483,674.08 €	26,801,361.08 €
Profits after taxes	78,508,796.85 €	79,451,022.24 €	80,404,083.23 €
Interest of the loan	4,823,669.15 €	4,441,791.31 €	4,040,472.07 €
Loan payment	7,501,037.86 €	7,882,915.70 €	8,284,234.94 €
Accumulated loan payment	87,247,914.17 €	79,364,998.47 €	71,080,763.53 €
Cash Flow	71,007,758.98 €	71,568,106.54 €	72,119,848.29 €
Discounted cash flow	52,712,384.06 €	50,554,620.55 €	48,476,427.59 €
Accumulated Cash Flow	233,884,388.05 €	284,439,008.60 €	332,915,436.19 €

Table 9. Cash flow and other results (continuation). (Own authorship)

Year	9	10	11
Revenues (Incomes)	288,178,272.32 €	291,492,322.46 €	294,844,484.16 €
Fixed cost of production	-5,081,393.83 €	-5,139,829.86 €	-5,198,937.90 €
Variable costs of production	-170,040,944.21 €	-171,996,415.06 €	-173,974,373.84 €
Annual repayment	-4,565,128.39 €	-4,565,128.39 €	-4,565,128.39 €
Profits before taxes	108,490,805.90 €	109,790,949.14 €	111,106,044.03 €
Taxes	27,122,701.47 €	27,447,737.28 €	27,776,511.01 €
Profits after taxes	81,368,104.42 €	82,343,211.85 €	83,329,533.02 €
Interest of the loan	3,618,721.67 €	3,175,499.96 €	2,709,713.83 €
Loan payment	8,705,985.34 €	9,149,207.05 €	9,614,993.19 €
Accumulated loan payment	62,374,778.19 €	53,225,571.13 €	43,610,577.95 €
Cash Flow	72,662,119.08 €	73,194,004.80 €	73,714,539.84 €
Discounted cash flow	46,474,886.49 €	44,547,184.84 €	42,690,612.72 €
Accumulated Cash Flow	379,390,322.68 €	423,937,507.53 €	466,628,120.25 €

Table 10. Cash flow and other results (continuation). (Own authorship)

Year	12	13	14	15
Revenues (Incomes)	298,235,195.73 €	301,664,900.48 €	305,134,046.84 €	308,643,088.38 €
Fixed cost of production	-5,258,725.69 €	-5,319,201.03 €	-5,380,371.85 €	-5,442,246.12 €
Variable costs of production	-175,975,079.14 €	-177,998,792.55 €	-180,045,778.66 €	-182,116,305.11 €
Annual repayment	-4,565,128.39 €	-4,565,128.39 €	-4,565,128.39 €	-4,565,128.39 €
Profits before taxes	112,436,262.51 €	113,781,778.51 €	115,142,767.94 €	116,519,408.75 €
Taxes	28,109,065.63 €	28,445,444.63 €	28,785,691.98 €	29,129,852.19 €
Profits after taxes	84,327,196.89 €	85,336,333.88 €	86,357,075.95 €	87,389,556.56 €
Interest of the loan	2,220,214.52 €	1,705,794.81 €	1,165,185.99 €	597,054.78 €
Loan payment	10,104,492.49 €	10,618,912.20 €	11,159,521.02 €	11,727,652.24 €
Accumulated loan payment	33,506,085.46 €	22,887,173.26 €	11,727,652.24 €	0.00 €
Cash Flow	74,222,704.40 €	74,717,421.68 €	75,197,554.93 €	75,661,904.32 €
Discounted cash flow	40,902,558.93 €	39,180,507.50 €	37,522,034.21 €	35,924,803.27 €
Accumulated Cash Flow	507,530,679.17 €	546,711,186.67 €	584,233,220.88 €	620,158,024.15 €

4. Economic assessment of the project

4.1 Net present value (NPV)

The Net Present Value (NPV) is an accumulation of the investment and discounted cash flows and is based on the value of the money with time. Positive values for this method implies that this project is profitable and the capital costs are fully recovered. This method is based on the difference between present value of the net cash inflows and the cash outflows.

The net present value of this project can be estimated with equation 8. [6]

$$NPV = \sum_{i=1}^{i=n} \frac{C_n}{(1+i)^n} - C_o \tag{8}$$

Where,

NPV= Net present value.

C_o = Initial investment.

C_n= Cash flow for the considered year.

n = year of the project.

i = interest rate of return or discounting rate.

This project can be considered profitable from the Net Present Value point of view because the result obtained is positive. The result of the NPV is 408,888,733.90.

4.2 Internal return rate (IRR)

The internal rate of return is the discounting rate which matches the present value of the cash flows and the cash inflows. For this reason, the net present value is cero. This rate of return must be compared with the required rate of return in order to determine the viability of the project. The internal rate of return can be expressed algebraically as indicated in equation 9.

$$\sum_{i=1}^{i=n} \frac{C_n}{(1+i)^n} - C_o = 0 \tag{9}$$

The final result of the internal return rate is 49.5%. As the internal rate of return is high than the interest rate the project is viable.

4.3 Return period of investment (Payback)

The payback is defined as the period of time for the recovery of the investment of a project. The payback is a simple method which empathizes on the liquidity of the project through the recovery of capital. The payback period is accepted when the value for the time of recovery is lower than a predetermined period or cut-off rate. Figure 1 specifies an approximate value for the payback. The accumulated cash flow is represented in the y-axis and the life period of the project in the x-axis. The point at which the curve crosses the x-axis is defined as payback. The value of the payback is approximately 1 year and 10 months.

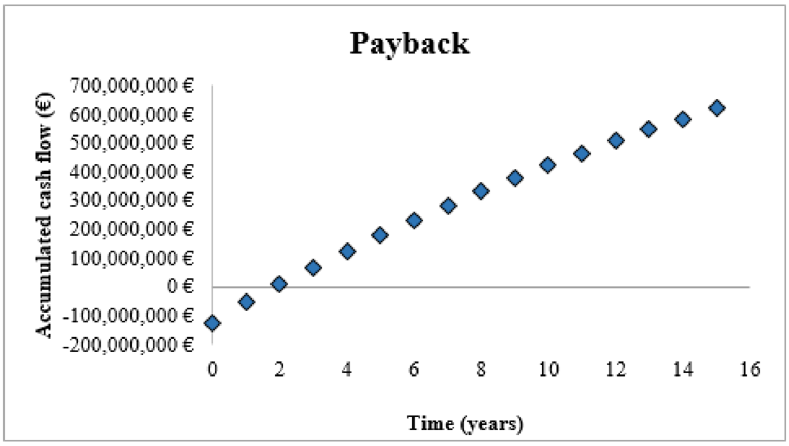

Figure 1. Representation for the payback. (Own authorship)

5. Sensitivity analysis

5.1 Introduction

The sensitivity analysis main objective is to perform an examination of the economic profitability of the project under different conditions. The analysis will be carried out taking two parameters and changing their conditions with respect to the current expected situation. The determining variables will be, then, the benefits and the investment of the project.

5.2 Analysis to the change of benefits

The polylactic acid is a new recent product with an increasing market. However, and because of competitiveness, the prices are different depending on the market region and type and purity of the polymer. A change of benefits includes, both, the increase or decrease of prices and the change in the sales. Figure 2 shows the relationship of the VAN with the change in benefits. More than 20% decrease of this parameter will become this project not profitable.

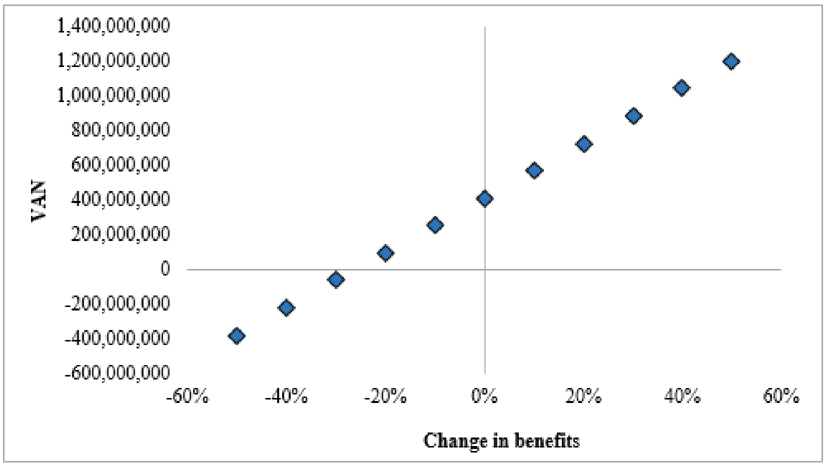

Figure 2. Analysis in the change of the benefits. (Own authorship).

5.3 Analysis to the change of investment

The capital required for the design and construction of a facility for the production of a polymer is pretty high. A normal facility for polymer production will require a capital cost in an approximate range of 10 to 200 million euros and sometimes may be higher. For these reason, the analysis over this parameter must be performed.

Table 11 illustrates the change of the VAN, TIR and payback for two variations in the capital investment. As expected, this parameter needs to be more significant in order to affect the project execution.

Table 11. Change of the capital. (Own authorship)

Change in capital	VAN	TIR	Payback
-20%	795,932,655.40	83.07%	1.22
20%	778,485,689.09	56.84%	1.88

6. Conclusion

This project is profitable, despite its high capital cost investment. However, a further analysis of the market and the prices of the polylactic acid will be needed. The price is a sensible parameter when determining the viability of the project.

This project has an expected very low payback. However, a decrease in the prices from 5,259.74 €/ton to 3,712.76 €/ton will sharply raise its value until 10 years.

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DOCUMENT II

Plans

INDEX

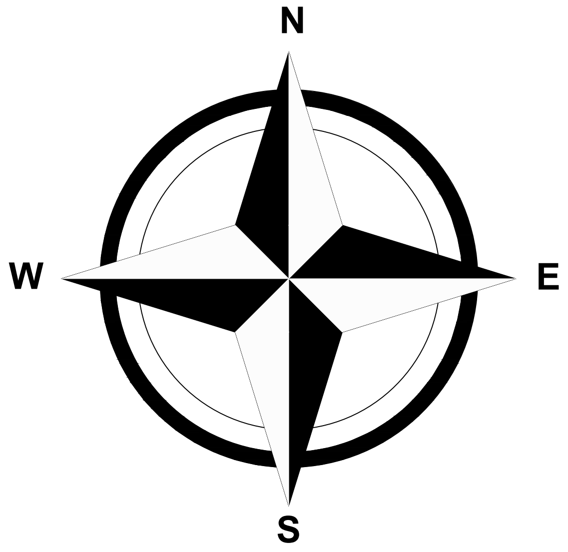
LEGEND

▨ Parc Sagunt I polygon approximate area

▨ Land plot approximate area

● Other locations of interest

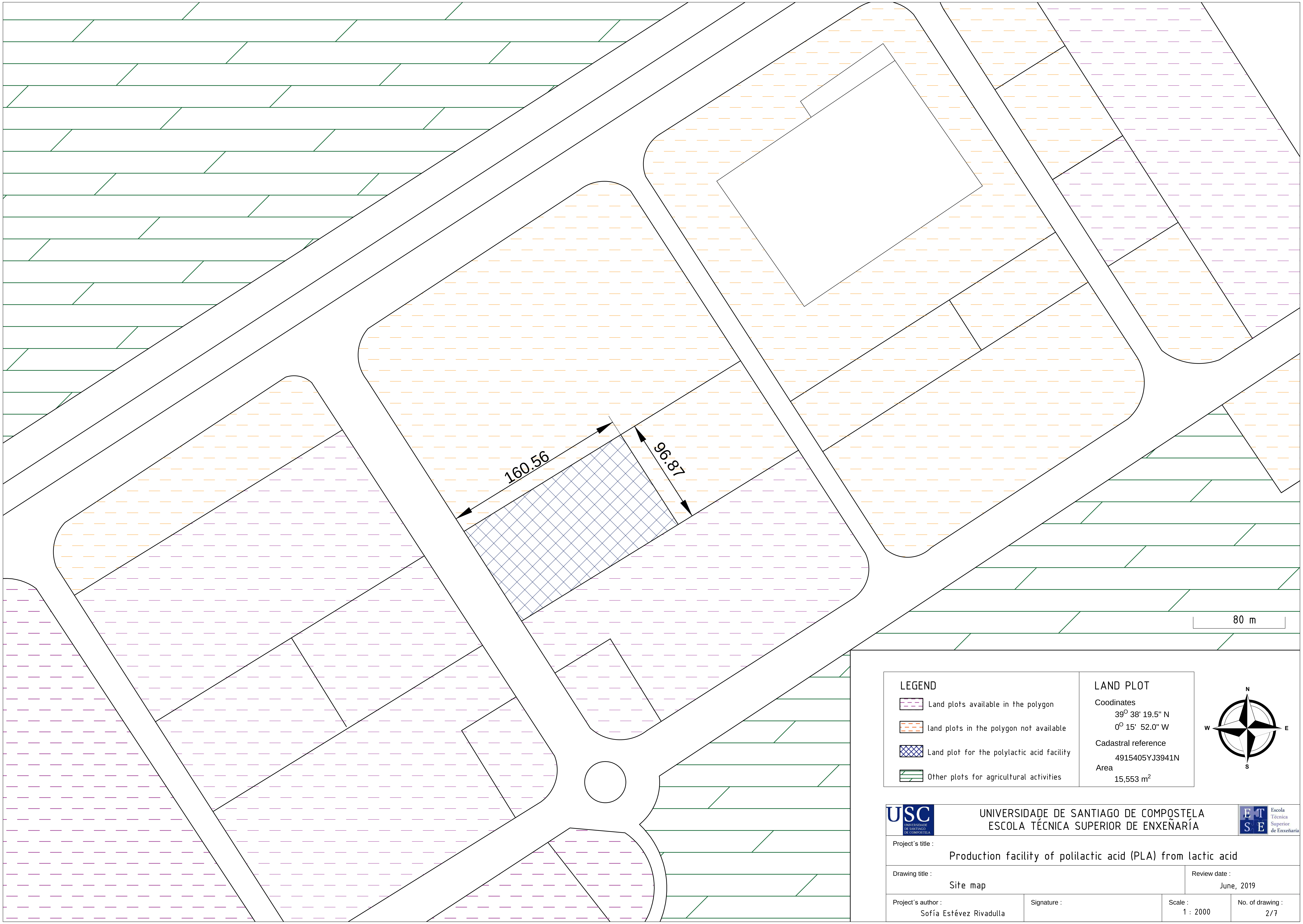
— Main roads



UNIVERSIDADE DE SANTIAGO DE COMPOSTELA
ESCOLA TÉCNICA SUPERIOR DE ENXEÑARÍA

Project´s title : Production facility of polilactic acid (PLA) from lactic acid	
Drawing title : Location map	Review date : June, 2019

Project´s author : Sofía Estévez Rivadulla	Signature :	Scale : 1 : 50000	No. of drawing : 1/7



LEGEND

🟪 Land plots available in the polygon

🟧 land plots in the polygon not available

▩ Land plot for the polylactic acid facility

🟩 Other plots for agricultural activities

LAND PLOT

Coodinates
39^{O} 38' 19.5" N
0^{O} 15' 52.0" W

Cadastral reference
4915405YJ3941N
Area
15,553 m^2

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ESCOLA TÉCNICA SUPERIOR DE ENXEÑARÍA

Project´s title :
Production facility of polilactic acid (PLA) from lactic acid

Drawing title :
Site map

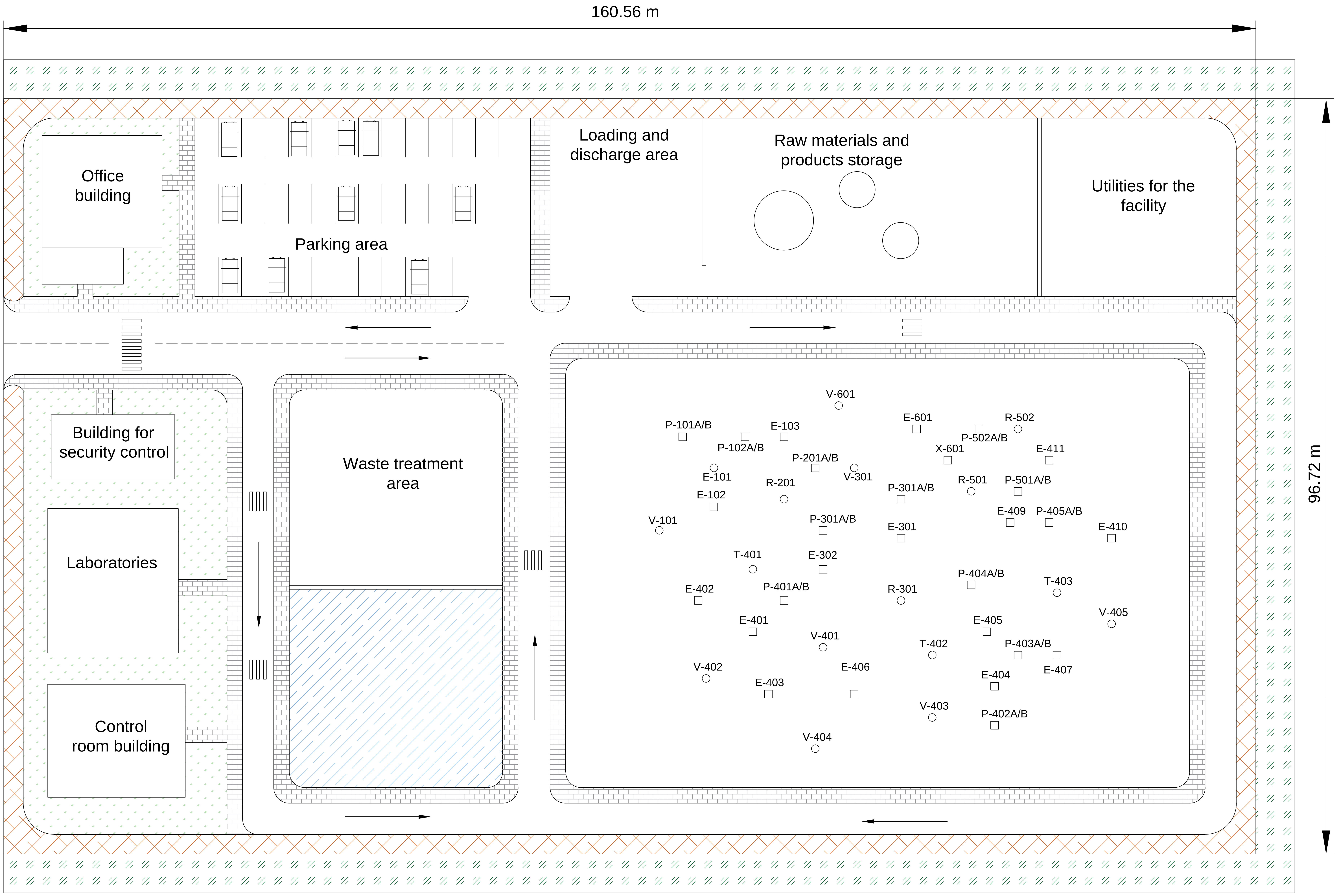
Review date :
June, 2019

Project´s author :
Sofía Estévez Rivadulla

Signature :

Scale :
1 : 2000

No. of drawing :
2/7



LEGEND

- 🟧 Limit walls and legal space of the facilities
- ▦ Sidewalks for pedestrians
- 🟦 Area for future expansions
- 🟩 Other land plots in the surroundings
- ░ Grass

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Project´s title : Production facility of polilactic acid (PLA) from lactic acid

Drawing title : Implementation Plan

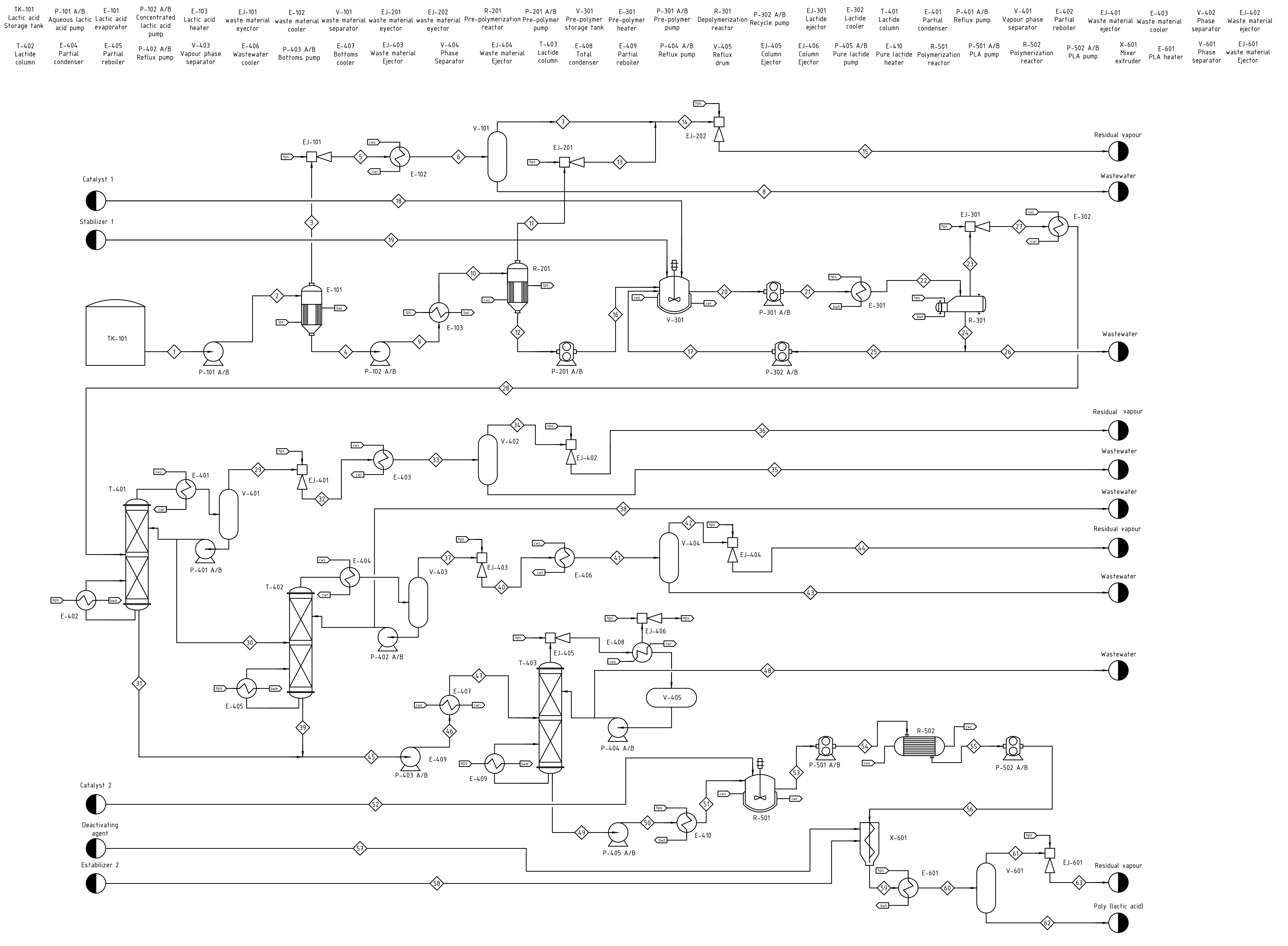
Review date : June, 2019

Project´s author : Sofía Estévez Rivadulla

Signature :

Scale : 1 : 350

No. of drawing : 3/7



Stream number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Temperature (ºC)	20	20	95	95	209	85	85	85	95	140	180	180	203	143.79	190.40	180
Pressure (bar)	1.013	1.013	0.065	0.065	0.5	0.5	0.5	0.5	0.35	0.35	0.35	0.35	0.5	0.5	1.01	0.35
Vapour fraction	0	0	1	0	1	0.68	1	0	0	0	1	0.01	1	1	1	0.01
Total mass flow (kg/h)	12970.71	12970.71	2984.18	9986.53	2984.18	2984.18	2027.04	957.14	9986.53	9986.53	1895.96	8090.57	1895.96	3922.99	3922.99	8090.57
Total molar flow (kmol/h)	249.73	249.73	132.52	117.216	132.52	132.52	103.55	28.96	117.216	117.216	105.07	15.120443	105.07	208.62	208.62	15.120443
Components mass flows (kg/h)																
L-Lactic acid	9857.74	9857.74	510.36	9347.37	510.36	510.36	5.47	504.90	9347.37	9347.37	0	504.57	0	5.47	5.47	504.57
D-Lactic acid	518.83	518.83	26.86	491.97	26.86	26.86	0.29	26.57	491.97	491.97	0	54.51	0	0.29	0.29	54.51
Water	2205.02	2205.02	2065.30	139.72	2065.30	2065.30	1662.92	402.38	139.72	139.72	1888.70	107.03	1888.70	3551.62	3551.62	107.03
Volatile impurities	388.91	388.91	381.65	7.26	381.65	381.65	358.36	23.29	7.26	7.26	7.26	0	7.26	365.62	365.62	0
Non-volatile impurities	0.21	0.21	0	0.21	0	0	0	0	0.21	0.21	0	0.21	0	0	0	0.21
Poly (lactic acid)	0	0	0	0	0	0	0	0	0	0	0	7424.26	0	0	0	7424.26
L-Lactide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
D-Lactide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Meso-Lactide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oligomers	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Catalyst 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Stabilizer	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Catalyst 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Deactivating reagent	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Stabilizer 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Stream number	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
Temperature (ºC)	220	20	20	160	160	220	220	220	220	220	232.1	120	112	112	152
Pressure (bar)	0.35	1.01	1.01	0.35	0.35	0.35	0.025	0.025	0.025	0.025	0.06	0.06	0.02	0.02	0.02
Vapour fraction	0	0	0	0.01	0.06	0.06	1	0	0	0	1	0.13	1	0	0
Total mass flow (kg/h)	3169.12	1.00	0.20	11260.89	11260.89	11260.89	7924.98	3335.91	3169.12	166.80	7924.98	7924.98	456.81	3931.36	3536.81
Total molar flow (kmol/h)	1.3344962	0.0025	0.0016	16.46	16.46	16.46	64.85	1.40	1.33	0.07	64.85	64.85	12.66	27.46	24.72
Components mass flows (kg/h)															
L-Lactic acid	0	0	0	504.57	504.57	504.57	75.69	0	0	0	75.69	75.69	6.38	29.10	40.20
D-Lactic acid	0	0	0	54.51	54.51	54.51	8.18	0	0	0	8.18	8.18	0.69	3.14	4.34
Water	0	0	0	107.03	107.03	107.03	202.07	0	0	0	202.07	202.07	196.50	5.57	0
Volatile impurities	0	0	0	0	0	0	0	0	0	0	0	0.00	0	0	0
Non-volatile impurities	3.94	0	0	4.15	4.15	4.15	0	4.15	3.94	0.21	0	0.00	0	0	0
Poly (lactic acid)	3142.38	0	0	10566.64	10566.64	10566.64	0	3307.76	3142.38	165.39	0	0.00	0	0	0
L-Lactide	0	0	0	0	0	0	5793.36	0	0	0	5793.36	5793.36	118.56	2884.71	2790.09
D-Lactide	0	0	0	0	0	0	625.88	0	0	0	625.88	625.88	12.81	311.64	301.42
Meso-Lactide	0	0	0	0	0	0	832.12	0	0	0	832.12	832.12	17.03	414.34	400.75
Oligomers	0	0	0	0	0	0	387.69	0	0	0	387.69	387.69	104.84	282.85	0
Catalyst 1	19.0	1.0	0	20.0	20.0	20.0	0	20.0	19.00	1.00	0	0	0	0	0
Stabilizer	3.80	0	0.2	4.0	4.0	4.0	0	4.0	3.80	0.20	0	0	0	0	0
Catalyst 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Deactivating reagent	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Stabilizer 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

LEYEND SHEET

UTILITIES NOMENCLATURE

lps	Low pressure steam
mps	Medium pressure steam
hps	High pressure steam
bwh	Boiler feed water, high pressure
bwm	Boiler feed water, medium pressure
bwl	Boiler feed water, low pressure
cws	Cooling water supply
cwr	Cooling water return

NOTES

1. The flow rate for utilities for ejectors were not included in the table for balances
2. Special notation for extruder X-601.
3. Null values in the balance table are without decimals.
4. Catalyst 1 is stannous octoate.
5. Stabilizer 1 is trimethyl phosphite.
6. Catalyst 2 is a mixture of stannous octoate and 1-dodecanol.
7. Deactivating agent is phosphoric acid.
8. Stabilizer 2 is 2,6-di-t-butyl-4-methylphenol.

SYMBOLS IN THE DIAGRAM

◐ Process stream output

◑ Process stream input

◇ Stream number

EQUIPMENT IDENTIFICATION

Section 100

TK-101	Tank
P-101 A/B	Pump
E-101	Evaporator
P-102 A/B	Pump
E-103	Heat exchanger
EJ-101	Ejector
E-102	Heat exchanger
V-101	Separator

Section 200

EJ-201	Ejector
EJ-202	Ejector
R-201	Reactor
P-201 A/B	Pump

Section 300

V-301	Vessel
E-301	Heat exchanger
P-301 A/B	Pump
R-301	Reactor
P-302 A/B	Pump
EJ-301	Ejector
E-302	Heat exchanger

Section 500

R-501	Reactor
P-501 A/B	Pump
R-502	Reactor
P-502 A/B	Pump

Section 400

T-401	Column
E-401	Condenser
P-401 A/B	Pump
V-401	Separator
E-402	Reboiler
EJ-401	Ejector
V-402	Separator
EJ-402	Ejector
T-402	Column
E-404	Condenser
E-405	Reboiler
P-402 A/B	Pump
V-403	Separator
P-403 A/B	Pump
E-407	Heat exchanger
EJ-403	Ejector
V-404	Separator
T-403	Column
E-408	Condenser
E-409	Reboiler
P-404	Pump
V-405	Reflux drum
EJ-405	Ejector
EJ-406	Ejector
P-405 A/B	Pump
E-410	Heat exchanger
E-403	Heat exchanger
E-406	Heat exchanger

Section 600

X-601	Extruder	V-601	Separator
E-601	Heat exchanger	EJ-601	Ejector

UNIVERSIDADE DE SANTIAGO DE COMPOSTELA
ESCOLA TÉCNICA SUPERIOR DE ENXEÑARÍA

Project´s title :
Production facility of polilactic acid (PLA) from lactic acid

Drawing title :
Process Flow Diagram I (PFD)

Review date :
June, 2019

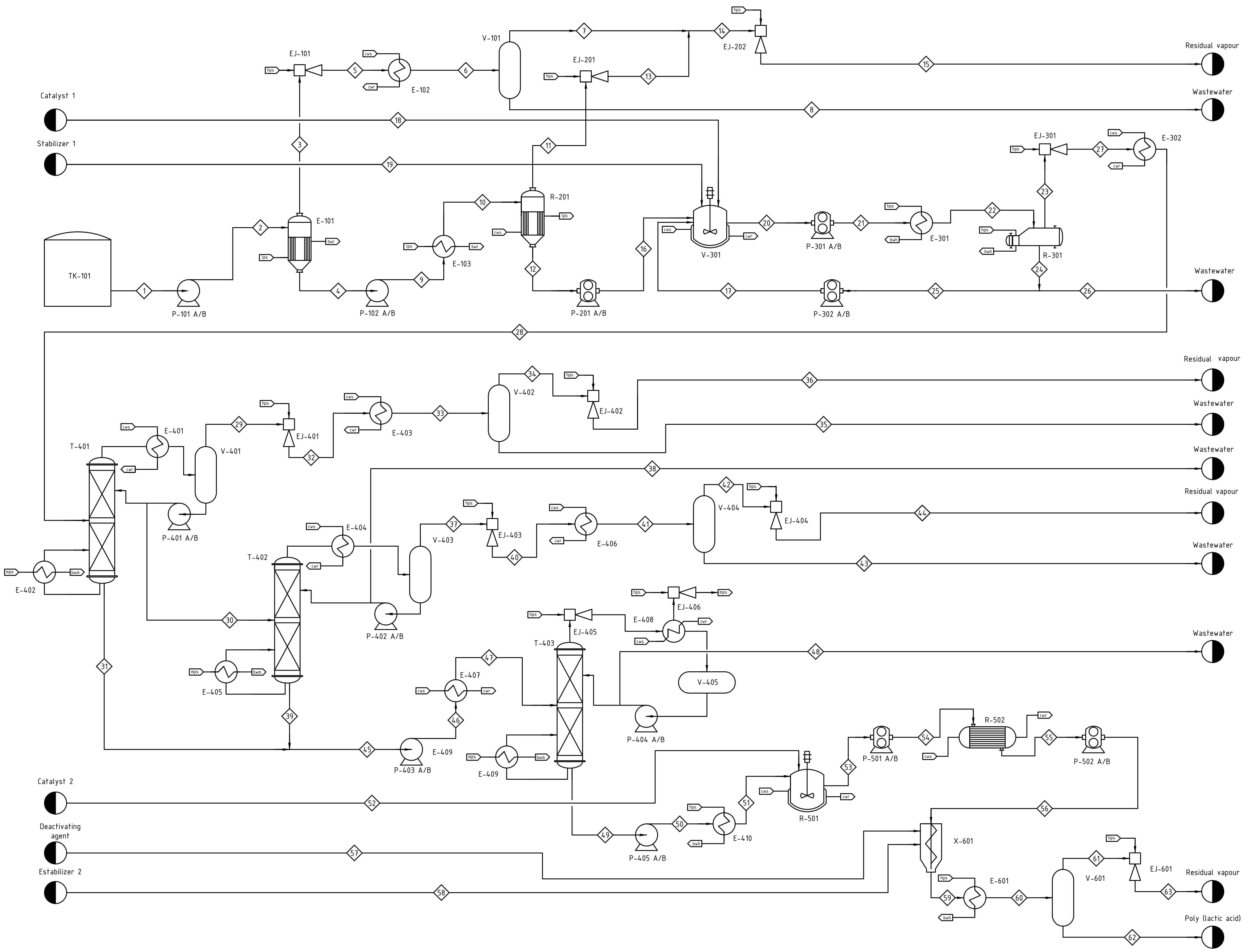
Project´s author :
Sofía Estévez Rivadulla

Signature :

Scale :
S/E

No. of drawing :
4/7

TK-101	Lactic acid Storage tank
P-101 A/B	Aqueous lactic acid pump
E-101	Lactic acid evaporator
P-102 A/B	Concentrated lactic acid pump
E-103	Lactic acid heater
EJ-101	waste material eyector
E-102	waste material cooler
V-101	waste material separator
EJ-201	waste material eyector
EJ-202	waste material eyector
R-201	Pre-polymerization reactor
P-201 A/B	Pre-polymer pump
V-301	Pre-polymer storage tank
E-301	Pre-polymer heater
P-301 A/B	Pre-polymer pump
R-301	Depolymerization reactor
P-302 A/B	Recycle pump
EJ-301	Lactide ejector
E-302	Lactide cooler
T-401	Lactide column
E-401	Partial condenser
P-401 A/B	Reflux pump
V-401	Vapour phase separator
E-402	Partial reboiler
EJ-401	Waste material ejector
E-403	Waste material cooler
V-402	Phase separator
EJ-402	Waste material ejector
T-402	Lactide column
E-404	Partial condenser
E-405	Partial reboiler
P-402 A/B	Reflux pump
V-403	Vapour phase separator
E-406	Wastewater cooler
P-403 A/B	Bottoms pump
E-407	Bottoms cooler
EJ-403	Waste material Ejector
V-404	Phase Separator
EJ-404	Waste material Ejector
T-403	Lactide column
E-408	Total condenser
E-409	Partial reboiler
P-404 A/B	Reflux pump
V-405	Reflux drum
EJ-405	Column Ejector
EJ-406	Column Ejector
P-405 A/B	Pure lactide pump
E-410	Pure lactide heater
R-501	Polymerization reactor
P-501 A/B	PLA pump
R-502	Polymerization reactor
P-502 A/B	PLA pump
X-601	Mixer extruder
E-601	PLA heater
V-601	Phase separator
EJ-601	waste material Ejector



Stream number	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**	**46**	**47**	**48**	**49**	**50**	**51**	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**	**61**	**62**	**63**
Temperature (ºC)	204.49	112	112	112	216.26	112	112	153.6	197.94	112	112	112	183.35	152.77	152.77	120	132.97	141.82	141.82	180	20	180	180	180	180	20	20	180	220	220	220	220
Pressure (bar)	0.02	0.15	0.15	0.15	1.01	0.02	0.02	0.02	0.15	0.15	0.15	0.15	1.01	0.02	0.02	0.02	0.02	0.02	0.3	0.3	1.01	0.3	0.3	0.3	0.3	1.01325	1.01325	0.3	0.3	0.065	0.065	1.01
Vapour fraction	1	0.54	1	0	0.76	1	0	0	1	0.2305025	1	0	0.53	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0508709	1	0	0
Total mass flow (kg/h)	456.81	456.81	248.66	208.15	248.66	34.52	606.94	3289.90	34.52	34.52	7.96	26.56	7.96	6826.71	6826.71	6826.71	820.71	6006.00	6006.00	6006.00	7.85	6013.85	6013.85	6013.85	6013.85	0.00	0.50	6014.35	6014.35	305.96	5708.39	305.96
Total molar flow (kmol/h)	12.66	12.66	11.11	1.56	11.11	0.47	4.13	22.87	0.47	0.47	0.28	0.19	0.28	47.59	47.59	47.59	5.92	41.67	41.67	41.67	0.04	22.63	22.63	2.15	2.15	0.00	0.00	2.15	2.15	2.11	0.04	2.11
Components mass flows (kg/h)																																
L-Lactic acid	6.38	6.38	1.82	4.56	1.82	1.07	18.74	9.30	1.07	1.07	0.08	0.98	0.08	49.50	49.50	49.50	49.50	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
D-Lactic acid	0.69	0.69	0.20	0.49	0.20	0.12	2.02	1.00	0.12	0.12	0.01	0.11	0.01	5.35	5.35	5.35	5.35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	196.50	196.50	193.66	2.84	193.66	5.02	0.55	0	5.02	5.02	4.69	0.33	4.69	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Volatile impurities	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Non-volatile impurities	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Poly (lactic acid)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2756.98	2756.98	5707.88	5707.88	0	0	5707.88	5707.88	0	5707.88	0
L-Lactide	118.56	118.56	8.22	110.34	8.22	2.79	261.73	2620.19	2.79	2.79	0.04	2.75	0.04	5410.28	5410.28	5410.28	44.07	5366.21	5366.21	5366.21	0	2903.01	2903.01	266.45	266.45	0	0	266.45	266.45	266.45	0	266.45
D-Lactide	12.81	12.81	0.89	11.92	0.89	0.30	28.28	283.07	0.30	0.30	0.00	0.30	0.00	584.49	584.49	584.49	4.76	579.73	579.73	579.73	0	313.62	313.62	28.79	28.79	0	0	28.79	28.79	28.79	0	28.79
Meso-Lactide	17.03	17.03	1.18	15.85	1.18	0.40	37.59	376.35	0.40	0.40	0.01	0.39	0.01	777.10	777.10	777.10	717.04	60.06	60.06	60.06	0	32.49	32.49	2.98	2.98	0	0	2.98	2.98	2.98	0	2.98
Oligomers	104.84	104.84	42.69	62.15	42.69	24.82	258.03	0	24.82	24.82	3.12	21.70	3.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Catalyst 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Stabilizer	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Catalyst 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7.85	7.85	7.85	7.74	7.74	0	0	7.74	7.74	7.73	0.01	7.73
Deactivating reagent	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00092	0	0.00092	0.00092	0.00092	0	0.00092
Stabilizer 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5	0.5	0	0.5	0

LEYEND SHEET

UTILITIES NOMENCLATURE

lps	Low pressure steam
mps	Medium pressure steam
hps	High pressure steam
bwh	Boiler feed water, high pressure
bwm	Boiler feed water, medium pressure
bwl	Boiler feed water, low pressure
cws	Cooling water supply
cwr	Cooling water return

NOTES

1. The flow rate for utilities for ejectors were included in the table for balances
2. Special notation for extruder X-601.
3. Null values in the balance table are without decimals.
4. Catalyst 1 is stannous octoate.
5. Stabilizer 1 is trimethyl phosphite.
6. Catalyst 2 is a mixture of stannous octoate and 1-dodecanol.
7. Deactivating agent is phosphoric acid.
8. Stabilizer 2 is 2,6-di-t-butyl-4-methylphenol.

SYMBOLS IN THE DIAGRAM

◐ Process stream output

◑ Process stream input

◇ Stream number

EQUIPMENT IDENTIFICATION

Section 100

TK-101	Tank
P-101 A/B	Pump
E-101	Evaporator
P-102 A/B	Pump
E-103	Heat exchanger
EJ-101	Ejector
E-102	Heat exchanger
V-101	Separator

Section 200

EJ-201	Ejector
EJ-202	Ejector
R-201	Reactor
P-201 A/B	Pump

Section 300

V-301	Vessel
E-301	Heat exchanger
P-301 A/B	Pump
R-301	Reactor
P-302 A/B	Pump
EJ-301	Ejector
E-302	Heat exchanger

Section 500

R-501	Reactor
P-501 A/B	Pump
R-502	Reactor
P-502 A/B	Pump

Section 400

T-401	Column
E-401	Condenser
P-401 A/B	Pump
V-401	Separator
E-402	Reboiler
EJ-401	Ejector
V-402	Separator
EJ-402	Ejector
T-402	Column
E-404	Condenser
E-405	Reboiler
P-402 A/B	Pump
V-403	Separator
P-403 A/B	Pump
E-407	Heat exchanger
EJ-403	Ejector
V-404	Separator
T-403	Column
E-408	Condenser
E-409	Reboiler
P-404	Pump
V-405	Reflux drum
EJ-405	Ejector
EJ-406	Ejector
P-405 A/B	Pump
E-410	Heat exchanger
E-403	Heat exchanger
E-406	Heat exchanger

Section 600

X-601	Extruder
E-601	Heat exchanger
V-601	Separator
EJ-601	Ejector

UNIVERSIDADE DE SANTIAGO DE COMPOSTELA
ESCOLA TÉCNICA SUPERIOR DE ENXEÑARÍA

Project´s title :
Production facility of polilactic acid (PLA) from lactic acid

Drawing title :
Process Flow Diagram II (PFD)

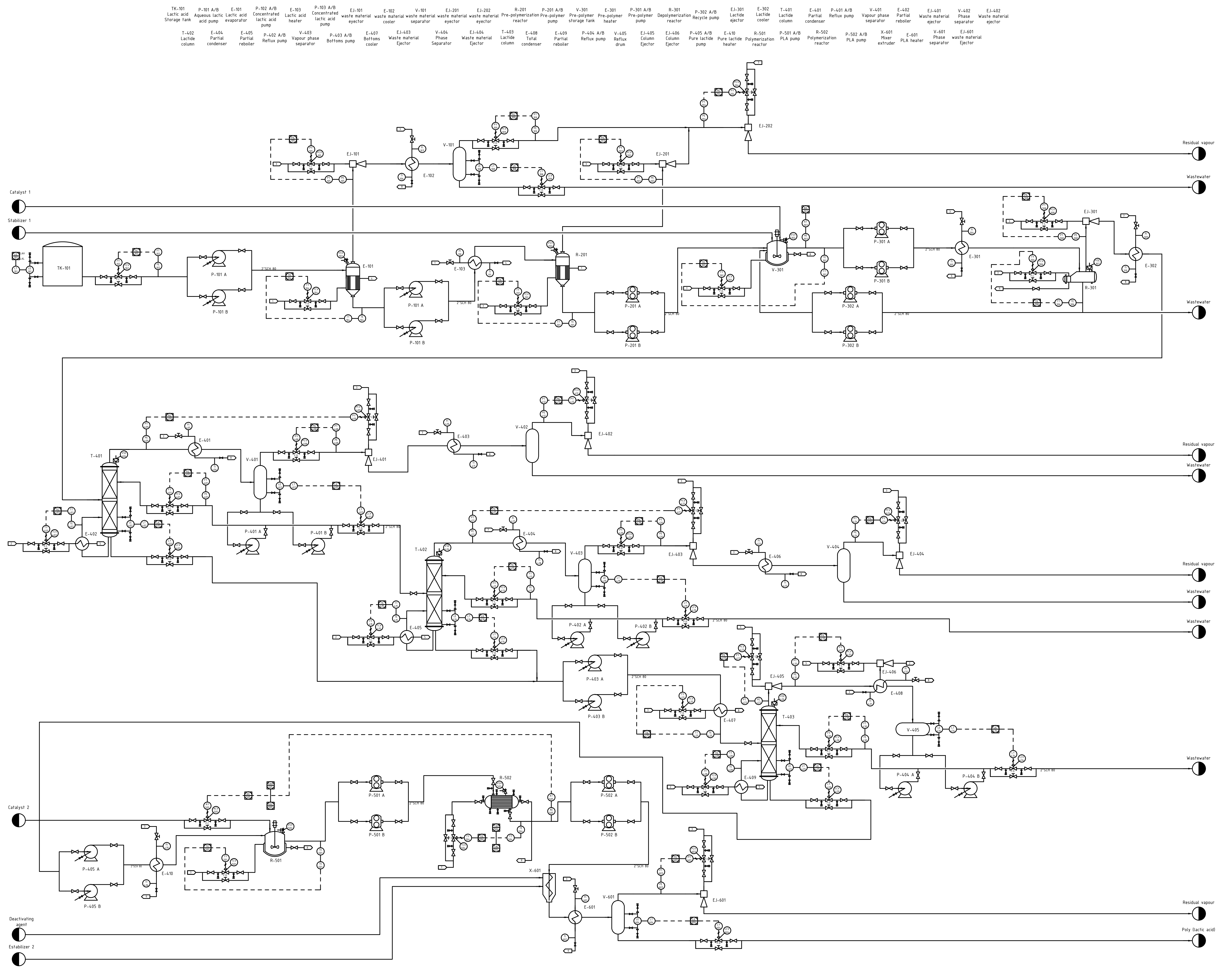
Review date :
June, 2019

Project´s author :
Sofía Estévez Rivadulla

Signature :

Scale :
S/E

No. of drawing :
5/7



LEYEND SHEET

UTILITIES NOMENCLATURE

1	Low pressure steam (lps)
2	Medium pressure steam (mps)
3	High pressure steam (hps)
4	Boiler feed water, low pressure (bwl)
5	Boiler feed water, medium pressure (bwm)
6	Boiler feed water, low pressure (bwh)
7	Cooling water supply (cws)
8	Cooling water return (cwr)

INSTRUMENT AND LINE SYMBOLS

Process line

Electric signal

Pneumatic signal

INSTRUMENT IDENTIFICATION

Analysis	AE	-	AT	AIC	AY	ACV
Flow rate	FE	FI	FT	FIC	FY	FCV
Temperature	TE	TI	TT	TIC	TY	TCV
Pressure	PE	-	PT	PIC	PY	PCV
Level	LE	-	LT	LIC	LY	LCV

SYMBOLS FOR VALVES AND OTHERS

Automatic valve

Valve (not especified)

Drainage valve

Relief valve

Rupture disc

EQUIPMENT IDENTIFICATION

Section 100

TK-101	Tank
P-101 A/B	Pump
E-101	Evaporator
P-102 A/B	Pump
E-103	Heat exchanger
EJ-101	Ejector
E-102	Heat exchanger
V-101	Separator

Section 200

EJ-201	Ejector
EJ-202	Ejector
R-201	Reactor
P-201 A/B	Pump

Section 300

V-301	Vessel
E-301	Heat exchanger
P-301 A/B	Pump
R-301	Reactor
P-302 A/B	Pump
EJ-301	Ejector
E-302	Heat exchanger

Section 500

R-501	Reactor
P-501 A/B	Pump
R-502	Reactor
P-502 A/B	Pump

Section 600

X-601	Extruder
E-601	Heat exchanger
V-601	Separator
EJ-601	Ejector

Section 400

T-401	Column
E-401	Condenser
P-401 A/B	Pump
V-401	Separator
E-402	Reboiler
EJ-401	Ejector
V-402	Separator
EJ-402	Ejector
T-402	Column
E-404	Condenser
E-405	Reboiler
P-402 A/B	Pump
V-403	Separator
P-403 A/B	Pump
E-407	Heat exchanger
EJ-403	Ejector
V-404	Separator
T-403	Column
E-408	Condenser
E-409	Reboiler
P-404	Pump
V-405	Reflux drum
EJ-405	Ejector
EJ-406	Ejector
P-405 A/B	Pump
E-410	Heat exchanger
E-403	Heat exchanger
E-406	Heat exchanger

UNIVERSIDADE DE SANTIAGO DE COMPOSTELA
ESCOLA TÉCNICA SUPERIOR DE ENXEÑARÍA

Project´s title :
Production facility of polilactic acid (PLA) from lactic acid

Drawing title :
Piping and Intrumentation diagram (P&ID)

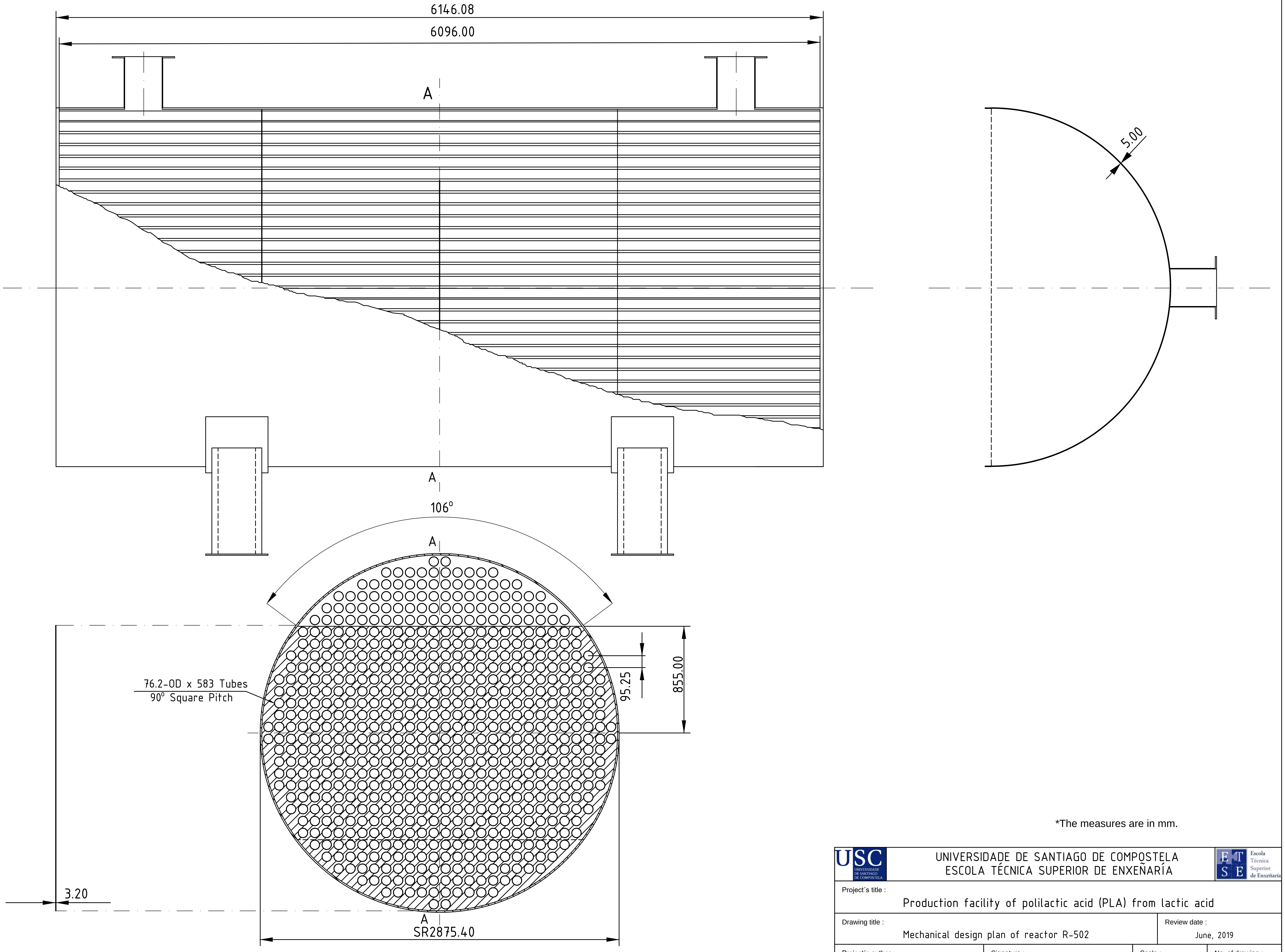
Review date :
June, 2019

Project´s author :
Sofía Estévez Rivadulla

Signature :

Scale :
S/E

No. of drawing :
6/7



*The measures are in mm.

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ESCOLA TÉCNICA SUPERIOR DE ENXEÑARÍA

Project´s title :
Production facility of polilactic acid (PLA) from lactic acid

Drawing title :
Mechanical design plan of reactor R-502

Review date :
June, 2019

Project´s author :
Sofía Estévez Rivadulla

Signature :

Scale :
1 : 20

No. of drawing :
7/7

DOCUMENT III

Self-Supporting Studies

Environmental impact assessment report

Index

1. Environmental Impact Assessment Report (EIAR)

1.1 Description of the project

1.1.1 Objective of the Study

An environmental impact assessment (EIA from now on) is a procedure that ensures the environmental effects examination for a project. This assessment is required for work and operation authorizations approval and is undertaken taken as basis the directive 2011/92/EU and the law 21/2013 of 9 December about environmental assessment.

According to this law, the environmental aspects can be considered during the writing of an Impact Assessment Report (here shown). This document is written by the project´s developer and includes an evaluation of significant effects over the environment when the project is to be carried out. From the evaluation, some suitable preventive measures can be taken.

The EIA main purpose is to provide a high level of protection for the environment from the very beginning of a project. It is an instrument to avoid environmental damage, so the identification, classification and study of the direct and side effects of an activity can be done. [1]

The PLA production facility from lactic acid is a project listed in Annex I in the law 21/2013. For this reason, this project is summited to an ordinary environmental assessment. The facility is classified inside group 5 (Chemical industry, petrochemical, textile and paper industry) according to Annex I and, in specific, for section a) and 1º part VIII (organic chemical products, plastic materials). This environmental impact assessment minimum contents for the previously named report are show in law 21/2013 in Annex VI.

1.1.2 Location of the project

The poly (lactic acid) facility can be located in the Valencia Community, and more particularly, in the province Valencia. The Sagunto´s region and municipality have been chosen for this location and in the area many polygons highlights, among them Parc Sagunt I is one of the most significant. Some characteristics are shown for the municipality location in table 1.

Table 1. Sagunto´s municipality characteristics location. [2]

Municipality average height (m)	45
Latitude values (in decimal degrees)	39.683º
Latitude values in degrees, min. and sec.	39º 41’ 0”
Longitude value (in decimal degrees)	-0.267º
Longitude value in degrees, min. and sec.	0º 16’ 0”
X UTM coordinates time zone 30	734418
Y UTM coordinates time zone 30	4396258.1
UTM grid	YJ39

The municipality is bordered to the north by Soneja Alfondequilla, Vall de Uxó, Almenara, Algar de Palancia, Cuart de les Valls, Benavites, Benifairó de los Valles y Faura; to the south by Puzol y El Puig; to the east by Canet de Berenguer y el mar Mediterráneo and to the west by Petrés, Gilet, Albalat de Taronchers, Torres Torres, Algimia de Alfara y Alfara de Algimia.

Parc Sagunt I, is the closer polygon with available land plots to the Sagunto´s port. The available and chosen plot is found in the following coordinates: 39º 38’ 19.5’’ N of latitude and 0º 15’ 52.0’’ W of longitude. More information about location and plot selection is on Document I. Descriptive report.

Figure 1 shows an aerial photography for the Parc Sagunt I polygon.

Figure 1. Aerial view of the Parc Sagunt I land plots. [3]

1.2 Environmental inventory

The environmental inventory is the set of factors in relation to the environment from which the conditions of the site can be deduced, so as the management of natural resources and the type of land occupation. This inventory is carried out before the building works of the project and includes a description of the factors of both biological-physical and socio-economical character.

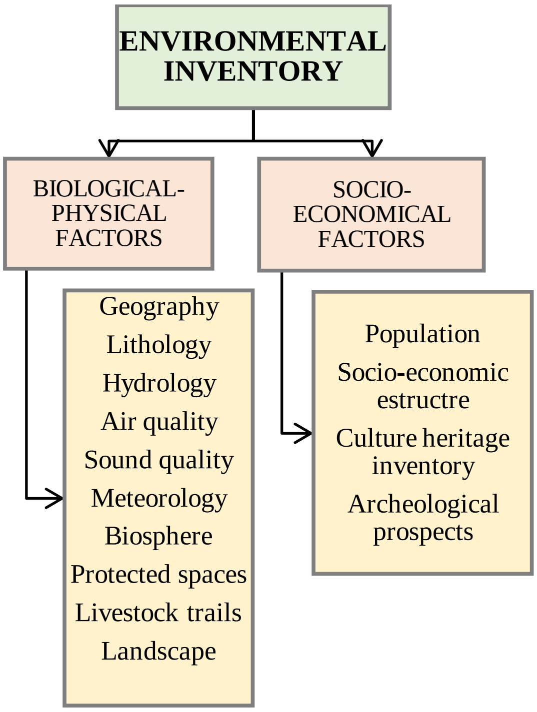


Figure 2. Headlines for an environment definition. (Own authorship)

1.2.1 Description of the biological-physical environment

This environmental impact assessment study section includes some environmental aspects and their characteristics, from which this project´s impacts can be examined. Accordingly, the following aspects are considered: geography, hydrology, lithology, air, biosphere and meteorology, so as other socio-economic aspects.

1.2.1.1 Geography, lithology (soil) and hydrology

Parc Sagunt I, is located in the municipal area of Sagunto, into Camp de Morvedre. This district has 271.10 km^2 and is placed in the north-east of the province of Valencia, which is located in the area named as Latin Mediterranean Arc. The hills sited nearby the Sagunto municipality have 200-300 m height, which decreases as long as it does the distance to the coastline. The Parc Sagun I polygon is located in an area with very flat terrain and the mountain systems are far from the facility location, about 6 km far away.

With regard to the lithology, the Sagunto municipality ground materials belong to ages between the Tertiary and Quaternary period. Most of them belong to the Mesozoic Era: Rodeno, limestone, carbonate sections and gypsum. Among the Tertiary Era materials are found some sandstones, conglomerates, Lucite with insertions of carbonates. The Quaternary Era materials are located near the coastline. The lithology composition is pebbles, gravel and silts nearby to the land plot location.

Apart from that, the hydrology is also significant. A hydrological study reflects the waters distribution and movement all over the surface and in the underground waters.

Figure 3. Hydrology in the surroundings of the Parc Sagunt I polygon. [4]

The hydrological network makes up of surface waters. This network consists of the Palancia river, which is 85 km length and has a 911.3 km^2 draining basin. This river is regulated by the reservoirs Regajo (6 Hm^3) and the Algar dam and passes through East to West with very irregular regime which is strongly influenced by the rainfalls. The flow rate differs during dry seasons and wet seasons (great increase after rainfalls). In this network there is also gullies and other watercourses with short courses, high gradient and irregular regime. Most of them remain dry during most part of the year. The annual catchment rate is estimated at 70 Hm^3/year.

The underground Waters can be classified into two mayor hydrological subsystems: Plana de Sagunto subsystem and Media de Palancia subsystem. The first appointed subsystem annual catchment rate reaches 104 Hm^3/year. The water release is produced by irrigations, urban and industrial extractions (82.6 Hm^3/year) and drains. The Media de Palancia subsystem is located in the middle of the Palancia river and has an area of 478 km^2 in the northeast in the Valencia province. This subsystem recharge is due to percolations, which are difficult to quantify because the Palancia river remains dry a great part of the year. The subsystem discharge is carried out through springs. Some are: San José, Quart, La Llosa, Almenara, Árguenes and Soneja. The springs can remain with flowrate during dry seasons.

Some examples of underground waters in the area are: Salto Caballo aquifer, Algar-Quart aquifer, Estivella aquifer, Gausa aquifer, Buntsandstein aquifer... The last one is the aquifer with the greatest capacity.

Some of the Sagunto municipality aquifers experience sea intrusion problems. The main reason is the aquifers overexploitation. In general, the aquifers have a flow direction to the sea but the direction can reverse due to this overexploitation and the underground waters composition can change increasing the sodium chloride salts. The mayor areas affected are the Parc Sagunt and the hillside of the Canet water reservoir.

In addition to all this, there is a serious risk of flooding in the Sagunto´s port facilities, which may affect the urban core of the area. [5]

The hydrology combined with the lithology and the topography are some aspects with a strong relationship with the construction processes. [6]

1.2.1.2 Air quality

The air quality touch upon the air conditions in relation the concentration of certain pollutants of interest. This parameter must be regularly under control (daily) and the monitoring activity is performed by a measument networks located all over the country. The evaluation is carried out according the Royal Decree 102/2011 of 28 January and the following compounds are considered: sulphur dioxide (SO_2), nitrogen dioxide y nitrous oxides (NO_2, NO_x), particles (PM_{10} y $PM_{2,5}$), lead (Pb), bencene (C_8H_8), carbon monoxide (CO), arsenic (As), cadmium (Cd), nickel (Ni), benzo(a)pyreno (B(a)P) y ozone (O_3).

The air quality can be evaluated with an adimensional air quality index (AQI) which value changes in a 0 to 500 range. As greater the quality index is, the greater the pollution and the health concern. A good air quality can be indicated with and air quality index lower than 50. In table 2 is shown the description associated with each one of the ranges of degree affectation for human health.

Table 2. Air Quality index description and ranges. [7]

Air Quality Index (AQI)	Value	Color	Description
Good	0-50	Green	Air quality satisfactory and air pollution present little or no risk.
Moderate	51-100	Yellow	Air quality acceptable. For some pollutants may be moderate health concern for a reduced group of people with unusual sensitivity to some pollutants.
Unhealthy for sensitive groups	101-150	Orange	Health concern for members of sensitive groups who may experience health effects. General public is not likely to be affected.
Unhealthy	151-200	Red	General public may begin experience health effects and sensitive members may experience serious health effects.
Very Unhealthy	201-300	Purple	Health alert. Everyone experiences serious health effects
Hazardous	301-500	Maroon	Emergency conditions. Everyone is likely to be affected.

Every day the pollutant concentration in the air is being measured. There is not a fixed value of the air quality index. However, the air quality used to be classified according the table 2 into good, moderate, unhealthy for sensitive persons… and used to depends on fixed factors which changes the air.

Table 3 shows data of the pollutant's concentrations for a specific day, 12 Mars 2019. There is also data of the maximum allowable concentrations in the air according to legislation.

Table 3. Air pollutant concentrations in 12 Mars 2019. [7]

Pollutant	Minimum measured value	Maximum measured value	Royal Decree 102/2011 maximum value concentrations	
$PM_{2.5}$	24	70	25	µg/m^3
PM_{10}	10	18	40	µg/m^3
O_3	1	43	120	µg/m^3
NO_2	2	35	40	µg/m^3
SO_2	2	7	350	µg/m^3
CO	0	0	10	mg/m^3

Sagunto´s greater contaminant is the particulate matter with a size lower than 2.5 μm. The maximum concentration reached in the indicated day was 70 $\mu g/m^3$, which is higher than the value established by the Royal Decree 102/2011.

The air quality index was 39. This value is in the range 0-50, so the quality of air is good.

1.2.1.3 Sound quality

The mayor sources of environmental noise in the Sagunto´s municipality have their origin on: the road traffic in the municipality, the road traffic in the urban center, the railway traffic coming from the industrial activity and leisure areas.

Nowadays, Sagunto does not have a noise map, enabling the sound levels to be identified for each municipality area. The main noise source among the previously appointed is traffic, the source with the greater acoustic impact. Most important among this are: The AP-7 motorway, V-21, V-23 and to a lesser extend CV-309, CV-314, CV-317, CV-320 and CV-329.

In industry, the sound levels are established by the Law 7/2002 of 3 December of the Generalitat Valenciana on protection against noise pollution. Thus, industrial areas must be located in where sound levels are not higher than 70 dB during the day and 60 dB on the night for the surroundings population. [8]

1.2.1.4 Meteorology

The Sagunto municipality meteorology can be described taking some climatic factors as basis: temperature, precipitation, wind, humidity and solar radiation.

- The climate

Sagunto has a typical Mediterranean climate. This climate characterizes by dry, hot summers and dry, soft and rainy winters. The rainfall is scarce and there are droughts during dry seasons. The annual average temperature is around 18ºC in spite of the hot summers with temperatures surpassing 38ºC. Sagunto municipality is located in the coastline, so the sea mitigates the climate factors with impact in the weather. [9]

- Solar radiation

The solar radiation is a climate contributor. It allows the air mass movement and facilitate the evaporation phenomena. Besides, it promotes the natural greenhouse effect. The climate is going to be warmer in areas where more solar energy reaches the ground. In Figure 4 is shown the solar energy quantification in kW/m^2 for different Spanish regions.

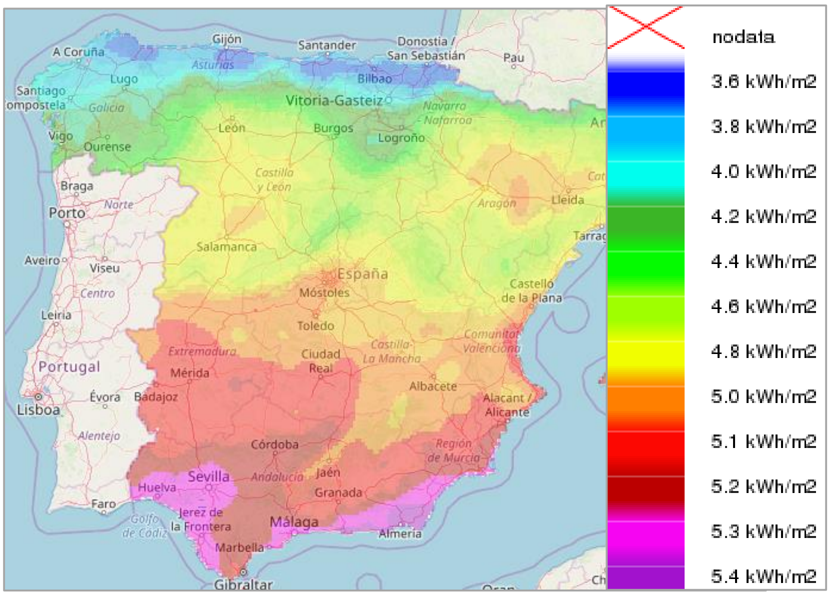


Figure 4. Solar irradiance map. [10]

- Temperatures

The Sagunto municipality has an average annual temperature of 16.05ºC. The coldest month (January) has an average temperature of 9.65ºC and the warmest month (august), 23.7ºC. The thermal range is about 11.56ºC.

- Precipitation

The average annual precipitation in the Sagunto municipality is 466.4 mm, which is lower to the 475 mm expected for Valencia City. This is because the territory is located downwind the zonal West current flow. October and July used to be the months with the largest and lowest precipitation respectively.

- Humidity

The relative humidity is between 62.2% and 69.4%.

- Wind

The prevailing winds in the Sagunto municipality are from the West (32.2% of the total wind direction) and the East (30.4% of the total). The wind is generally weak. [11]

1.2.1.5 Biosphere

- Flora

The Sagunto municipality land is widely used. There is a vast land expansion for agriculture and land development, compared to other minor land uses. The following distinguished areas are determined according to vegetation characteristics: irrigation areas, urban areas, seaside areas, hillside areas and wetlands.

In cultivation areas are found species like *Oxalis pes-Caprae, Portulaca oleracea, Piptatherum milaceum, ...*

In urban areas highlights: *Malva sylvestris, Urtica urens, Brachipodium retusum*, … There are also some exotic species like acacia, tuya, yucca, eucalyptus tree, … [5]

The hillside area is pretty weathered and bushes, woodland of pines and grasslands are predominant.

The seaside areas have the following species among others: *Pancratium maritimum, Echinophora spinosa, Cakile marítima, Eryngium maritimum* and *Elymus farctum*. [11]

The wetlands have a high biodiversity. The vegetation is distributed according the substrate salinity grade in: Nitrohalofile communities, hidrohalofile and freshwater lagoons. Some nitrohalofile species are *Glaucium flavum, Eryngium maritimum*, … Some hidrohalofile species are *Limonium dufourii* (endangered species), *Arthrocnemum fruticosum, Arthrocnemum macrostachyum*, … And inside freshwater lagoons are predominant *Phragmittes communis, Typha dominguensis* among others. [12]

- Wildlife

In the community of Valencia were recorded 12,201 species (in 2017): 511 species are vertebrates, 3,676 are invertebrates and the remaining species belonged to the vegetation. The Sagunto municipality has a total of 1,361 species. The kind of fauna living in the area depends on the flora and the habitat characteristics. For this reason, there are different species for diverse areas. [13]

The following species are found in cultivation regions: Little owl, Iberian Chiffchaff, Ash-Colored Lizard…There is also biodiversity in urban areas. Among reptiles can highlight geckos. There are some birds like the serin, the swallow, the robin, the common nightingale … And as invertebrate stands out bees, ants and wasps.

There are various types of shellfish and crustaceans: *Dona semistriatus* and skull crab *Portunis Latipes* respectively among others. These species are changing with the coastal line distance. Among insects is found the offshore fly *Fucelia maritimia* and among birds, Yellow-Legged Gulls, the Osprey, the Lark …

In mountain regions there are Orthoptera, Lepidoptera, Heteropteran and Coleoptera as insects, although there is also a great diversity of reptiles, amphibians, birds and mammals. Some examples for mammals are: *Suncus struscus, Rhinolophus ferrumequinum, Lepus Capensis* …

Some Cladocera can be watch in wet areas (marshlands), so as different types of fishes such as the *Murgil Caphalus* fish and different amphibian and reptile's species (*Prezi frog* and *Emys Orbicularys European turtle* respectively). There are some mammals: water rats, urchins, shrews, rabbits … Although in this habitat are vastly more abundant the birds. Some of them are being threaten: Marbled Teal, Ferruginous Duck and the aquatic Warbler. [5]

1.2.1.6 Protected Natural Spaces

The Sagunto´s municipality has diverse natural habitats, some of them deserving the implementation of conservation measures. A European ecological network named as "Natura 2000" has been created for habitats conservation. This network consists of different places with habitats compiled in Annex I and II of the Council Directive 92/43/CEE of 21 May 1992 on the conservation of natural habitats and of wild fauna and flora.

In the same way, the Law 42/2007 of 13 December on Natural Heritage and Biodiversity should also be taken into account. Pursuant to article 9 of this law, a Spanish natural heritage and biodiversity inventory is included and, according to article 30, natural protected spaces can be classified as: parks, natural reserves, marine protected areas, natural monuments and protected landscapes.

Under article 42, Natura 2000, as European ecologic network, consists of: Sites of Community Importance (SCI), Special Areas of Conservation (SPA) and Special Protection Areas for Birds (SPAB).

The natural protected spaces in Sagunto are: Natural Park of Sierra calderona, Marjal dels Moros, Marjal d´Almardà, Cova de sardiner, Marjal d´Almenara and Marjal i Estanys d´Almenara. There are also some micro-reserves as: Les Torberes d´Almardá, Camí de Rampete, Llacuna del Fartet, El Picaio, Marjal del Moros A and Marjal del Moros B.

There are 1,589.54 ha of total protected surface, which is a 11.97% of the total municipality surface. [14]

Marjals dels Moros is one of the most significant natural spaces together with Sierra Calderona. It is located between the municipal areas of Sagunto and Puçol, has 619.10 ha of land extension and is considered by the European Union as SCI, SPA and SPAB (included in Natura 2000), so as by the Decree 127/2015 of the Council of 31 July establishing Lavajos de Sinarcas, Marjal de Nules and Marjal dels Moros as Special Areas of Conservation (SPA) and Sites of Community Importance (SCI) and approving the management standards for those SCI and for Marjal dels Moros Special Protection Area for Birds (SPAB).

Despite this protected area has a small geographic extension, is one of the most important areas in the municipality due to the aquatic fauna. Among this, highlights the population of samaruc, farcet and the European pond turtle. It is a habitat for waterfowl breeding for species like the Marble Teal and Purple Swamphen and, until now, 230 bird's species have been recorded in the area.

As shown in figure 5, the Community of Valencia has different protected spaces. However, the humid zone of Marjal dels Moros has special interest due to the proximity to the Parc Sagunt I, in where this project´s facility is located.

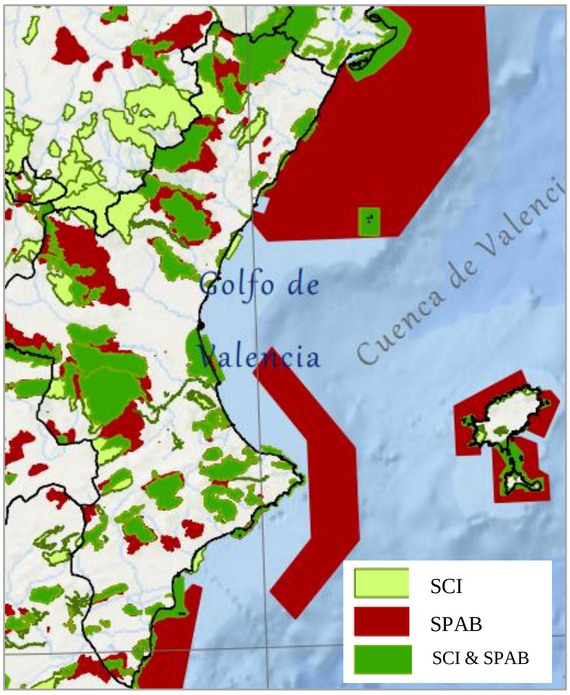


Figure 5. Natura 2000 network map for the community of Valencia. [15]

The delimitation of the frontiers of the Marjal dels Moros humid zone, so as the protection humid zone delimitation frontier, can be seen from figure 6.

Figure 6. Protected zone of Marjal dels Moros and livestock trails in the area. [4]

1.2.1.6 Livestock trail

The livestock trails are routes used by tradition for the migrating livestock. The Sagunto municipality has 3 livestock trails with 26,322 m length: *Cañada de Aragón o Camino de Liria* (with 7,479 m length), *Cañada de Gausa o Camino de Petrés* (with 6,501 m length) and *Cañada del Mar* (with 12,342 m length). These roads are protected by the Law 3/1995 of 23 Mars for livestock routes, which defines them as goods of public domain. The *Cañada del Mar* livestock route goes through Marjal dels Moros protected space and through the Sagunto´s port area. [16]

1.2.1.7 Landscape

Sagunto is subdivided into 7 well-differentiated areas in order to perform the study related to the location and landscape quality: build-up areas, beaches, industrial area, farming, Palancia river, Sierra Calderona and marshes. The landscape environmental quality must be evaluated for each of the landscape areas through its substantive visual quality. Sierra Calderona, the beaches and the marshes are the areas with the higher visual quality while the industrial areas have the poorest quality. According to the previously explained, there is a visual contrast between Parc Sagunt I and the protected space of Marjal dels Moros. [5]

1.2.2 Description of the social-economic environment

1.2.2.1 Population

The demography of the Sagunto municipality is going to be described in this environmental impact study section. The demography is a variable which has indirect relationship with other environmental aspects variables. In this sense, the demography affects the land occupation, the consumption of goods and natural resources and waste materials production. [5]

The Sagunto´s demography development is linked to the industrial economic development started in the XX century, which was the result of the establishment in the Sagunto´s port location of a steel industry. Accordingly, between 1920 and 1930, the population increases a 94.2%. Ever since the demography has shown a growth tendency, although in the last 20 years the tendency has not been much significant. [17]

Nowadays, the Sagunto municipality has 65,669 habitants (2018 data) and considering the 56,607 habitants living in Sagunto 20 years ago, the population has increased a 16%, which is an approximate annual increase of 0.8%. [18]

The Sagunto population, just like the rest of the Spanish population, is an ageing society and the population dynamics (as shown by the Sundberg demographic index indicator) may be considered as regressive. This is largely due to a 50 years old population being much greater than the 15 years old population. The birth rate, as indicated in 2016 data and expressed by the number of live births for every 1,000 habitants, is 8.2 and the death rate is 9.69. [19]

When it comes to the spatial population distribution, Sagunto has an approximate population density of 496.14 habitants/km^2 (data of 2018).

1.2.2.2 Socioeconomic structure

The Sagunto municipality has 3,543 enterprises (2016 data). The local economy is carried by the service sector, the 43.64% of the companies operates in this sector. The trading, transport and catering sector is another significant sector with a total weight in the economy of 40.73%. The building sector represents an 11.21% of the companies and the industrial sector is about a 4.43%. Each company provides a job post to the inhabitants of the area. Even so, the Camp de Morvedre district has a total of 6,249 non-employed persons. The 10.95% of the recorded people looking for employment is trained for works destined to the industrial sector, although the service sector is the one with the higher official figures for unemployed persons. The unemployment statistics seems to show a slight increase in the number of people without work in the industry sector. Agriculture and building sectors are the only one with positive statistics for workers. [20]

Another concept to take in mind in the local economy is the wealth. This parameter is measurable with the Gross Disposable Income per Inhabitant. The average income per capita in Sagunto is 23,619 euros, which is higher than the one expected for the Valencia Community, 23,006 euros. [21]

1.2.2.3 Cultural Heritage inventory

Sagunto has a wealth varied of artistic and historical heritage. Some Assets of Cultural Interests shown below:

- Monuments/ architectural heritage: There´s a total of 9 monuments. *Castillo de Sagunto, Teatro romano, Torre de San Roque, Museo Arqueológico del Teatro Romano, Molino Fortificado Torre Gausa, Iglesia Parroquial de la Natividad de Nuestra Señora, Fortín o Torre del Grau Vell, Iglesia Parroquial del Salvador y la Alquería Fortificada del Agua Fresca*. Some of the monuments previously named stand out for their special nature: *Castillo de Sagunto* and Sagunto´s *Teatro Romano.*
- Historic areas: The oldest area of the Sagunto town.
- Immaterial: *Sociedad Musical Lira Saguntina y Unión musical Porteña*.
- Archeological sites: *Grau Vell, Templo Diana* (megalithic remains of the Sagrario´s street) and *Villa Romana de Ponera*. [22]

1.2.2.4 Archaeological prospections

There are two mayor archaeological sites in Sagunto, which are important for their particular characteristics: *Grau Vell* and *Villa Romana de Ponera*.

The *Grau Vell* archaeological site, also named as *Puerto romano del Grau Vell,* was declared Asset of Cultural Interest according to the Decree 78/1992 of 11 May 1992 of the Government of Valencia. Nowadays, *Grau Vell* is considered to be the greatest maritime archaeological site in the Gulf of Valencia because of functioning tenth century port. The port can provide knowledge about maritime trade, navigation and harbor constructions. [23]

Another important archeological site is the *Villa Romana de Ponera* located in the Camp de Morvedre (Sagunto). This site significance lays on: the date of construction (50 B.C to 50 A.D.), the decorative program of the documented remains and the good pavement preservation. [24]

There is an archeological site inside the Parc Sagunt I polygon. Despite its significance is not comparable with the previously explained archeological sites, it must be taken into account due to proximity to the polylactic acid facility. The place is named as Alqueria del Abocata and it is a roman village of the second century A.D.

1.3 Environmental impacts

The effects over the environment of the industrial facilities implementation for this engineer basic project, located in the Sagunto municipality, is being described during this environmental impact assessment study section.

1.3.1 Actions with environmental impacts

The actions with potential for environmental effects production are being analyzed for each of the project´s phase. The project has 3 phases: construction, operation and decommissioning.

1.3.1.1 Construction phase

During the construction phase, perturbances on the following environmental compounds are produced: the meteorology, the air quality, the sound level, the soil characteristics, wildlife, vegetation and landscape.

The construction phase has scant importance on impacts on the weather and is associated with the equipment needed used during the building works. The equipment generates atmosphere emissions which deteriorates temporarily the air quality. There is also dust particle production in the works, which are found in suspension, due to land movements. The air quality would improve again once this phase ended.

Likewise, the equipment also increases the noise levels. The impact on the environment is, just like for air quality, temporal and discontinuous.

In the Sagunto municipality, and more specifically in the Parc Sagunt I area, there are not geological formations which deserves to be preserve. However, there are other soil characteristics to be considered, because these are becoming the soil into a pretty vulnerable environmental aspect.

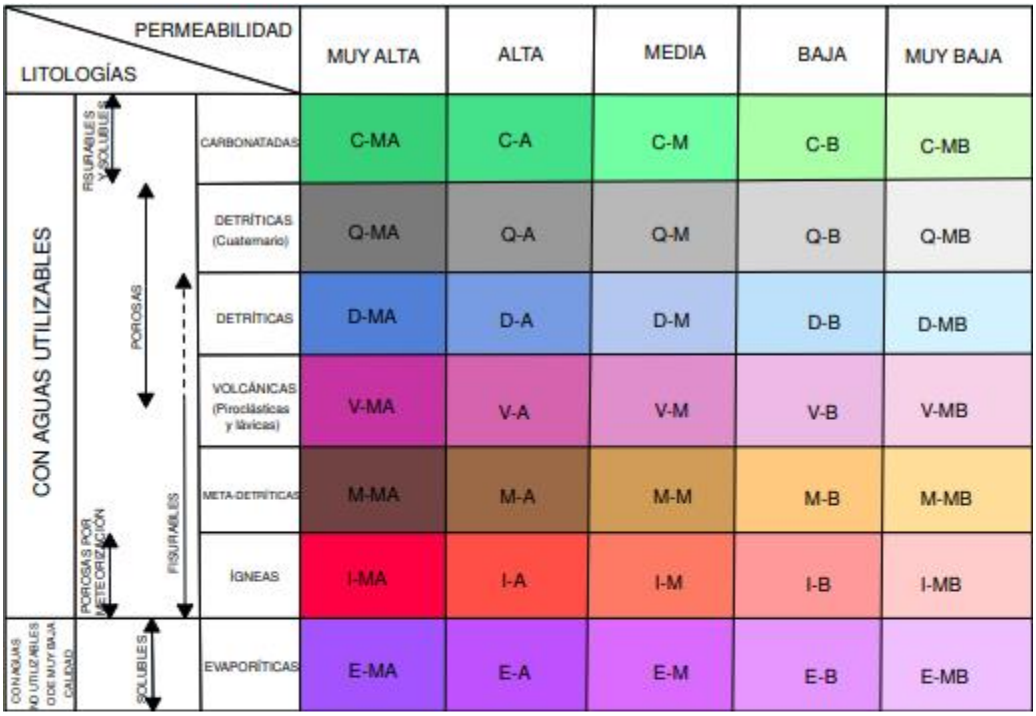
The soil is badly affected during the construction phase because of the land occupation (the installation can use a maximum of 15,553 m^2) and the next phenomena are produced: erosion, compaction, vegetation removal, … There are continuous land movements for conduction and equipment burials and for foundations, required for buildings and accesses.

The activities linked to this project phase have impacts on the soil with forest floor layers loss, soil contour desorganization due to land diggings and soil compactation which produces the permeability decrease and the creation of a physical barrier for revegetation. For all these reasons, the impacts on the soil are permanent and irrevocable.

The soil contour desorganization is irreversible, however, the effects over the landform are reversible. This effects can be corrected by restoring the gradient of the land to its initial state. Parc Sagunt I polygon infraestructure is already built and the land smoothed. The facility construction does no have impacts over the landform, nor do the access roads. The access roads inside the production facilities must be considered in order to determine impacts, but those located in the outside should not be take in mind.

The permeability, as previously explained, is an important characteristic of the soil. There can be oil and other wastes infiltrations due to equipment use during the construction phase. Infiltrations can pollute the soil, but also the underground waters. The main reason is a high permeability of the materials which forms the Sagunto´s municipality soil. In figures 7 and 8 is shown the permeability of the area. As explained in section 1.2.1.1, the materials belongs to the Quaternaty Era.

Figure 7. Permeability map. [25]



LITOLOGÍAS \ PERMEABILIDAD	MUY ALTA	ALTA	MEDIA	BAJA	MUY BAJA
CARBONATADAS	C-MA	C-A	C-M	C-B	C-MB
DETRÍTICAS (Cuaternario)	Q-MA	Q-A	Q-M	Q-B	Q-MB
DETRÍTICAS	D-MA	D-A	D-M	D-B	D-MB
VOLCÁNICAS (Piroclásticas y lávicas)	V-MA	V-A	V-M	V-B	V-MB
META-DETRÍTICAS	M-MA	M-A	M-M	M-B	M-MB
ÍGNEAS	I-MA	I-A	I-M	I-B	I-MB
EVAPORÍTICAS	E-MA	E-A	E-M	E-B	E-MB

Figure 8. Permeability map legend. [25]

Negative effects can also be produced on the flora during the construction phase. The existing vegetation is being removed, leading to erosive results in the superficial layers of the soil.

As a consequence of the flora elimination, the fauna can be harmed. The greenery acts as feeding and shelter for other living beings. The wildlife is also afected by the construction machinery noises, which disturb the resting conditions and induce the fauna getaway. This impact is temporary because once the contruction works comes to an end, it also does the impact.

Lastly, the landscape impact. There´s a scenery quality loss due to access setting up, diggins, foundations creation and selective cutting of vegetation.

However, during construction works, there are also positive impacts which are mainly in the socio economical field. The construction works creates new employment and demands services from the surrounding areas.

1.3.1.2 Operating phase

This phase begins once the facilities has been started-up. It can last for years, and therefore is the phase with greater long-term impact.

All industrial activities inevitably produce wastes, and the poly (lactic acid) production facility also does. The type and amount of generated wastes will be explained in the section 1.3.2 of this environmental impact study. Wastes have a fairly high environmental impact and might be liquids and vapor in these project.

The aqueous wastes produced modify the quality of the waters. Despite being under treatment before their disposal, the water composition and oxygenation is poorest compared to the environmental water in which is introduced. Furthermore, leaks must be taken in mind because of the possible filtrations in the land, which may affect the soil and underground waters quality.

During the facilities operation, there will be an increase on the noise level in the area. The noise can be produced by rubbing among gears, process equipment proper functioning and misfunctioning (pumps, compressors, heat exchangers,…), fluid flow in pipes, … As a consequence of the noise level increase, there will be a negative impact on the surroundings population and fauna. This last group has a special sensitivity and leave the area looking for a more appropriate habitat. This impact will last the facility useful life.

There are also socio-economic impacts. Some examples are: traffic increase in access roads due to staff and materials transport, so as machinery; generation of employment for people living in the closest urban centers, private land occupation which can be purchase or expropriated (for the construction of new access roads for example).

1.3.1.3 Decommissioning phase

This phase focuses on the production process finalization and the facilities dismantling. Similar activities to the previously explained in the construction process are being performed during the dismantling, hence the environmental impact is also similar. There will be, among other activities land movements and equipment, structures and foundations remain removal. The materials which result from the demolition works will be considered as wastes and will be submitted to subsequent treatment. For this reason, wastes should be stack in evacuation sites.

Finally, refurbishment works and habitat rehabilitation should be carried out: damage lands are restored to their original state. Land movements for the soil mixing in very compacted areas, fillings inclusion, reconstructions, soil replacements, soil landform correction, and decontamination are some activities for rehabilitation. Besides, reforestation programs can be prepared for the reestablishment of indigenous vegetation and desert land recovery. The final refurbishment has a very positive impact.

1.3.2 Waste materials, air emissions and other pollutants

This project is not characterized by air contaminant emissions, although accidental losses occurs. The great part of the waste streams are liquid or vapor, which can also be liquefied. The composition of the wastes depend on the stream of the process but the main contaminants are lactic acid, lactide, water, methanol and little fractions of catalysts.

The polylactic acid production facility produces a total of 58384.72 t/year from which 5258.84 t/year is lactic acid, 36302.57 is water, 3406.88 t/year and the rest is lactide. The catalyst lost can be consider negligible.

1.3.3 Impacts identification and classification

In section 1.3.1 has been introduced some environmental aspects. In this section the impacts identification is resumed synthetically and the impacts are classified. The criteria shown in tables 4 and 5 is taken into account for the classification.

Table 4. Classification category explanation for environmental impacts. [26]

Classification criterion	**Categories**
By the nature	**Simple impact:** The impact has effects on one single environmental aspect. **Cumulative impact:** The impact is increased when present and future actions are added to past actions. **Synergistic:** The impact is produced by the effect of several environmental agents. This environmental impact is greater than the addition of the individual impacts.
By cause-effect relationship	**Primary or direct:** Effects caused by an action happening at the same time and place. **Secondary or indirect:** Indirect changes induces in the environment.
By the time of onset	**Latent:** Impact which manifests after a certain time of the action beginning. **Immediate:** There is no time between the action beginning and the time the effects are detected. **Critical time:** Moment at which takes places the higher grade of impact.

Table 5. Classification category explanation for environmental impacts (Continuation). [26]

Classification criterion	Categories
By the interrelation between actions	**Simple impact:** The impact has effects on one single environmental aspect. **Cumulative impact:** The impact is increased when present and future actions are added to past actions. **Synergistic:** The impact is produced by the effect of several environmental agents. This environmental impact is greater than the addition of the individual impacts.
By the geographical extent	**Occasional:** The action having impacts on the environment produces a local disruption. **Partial:** The impact has a significant disturbance in the area. **Extreme:** The action produces a considerable deterioration of the land. **Total:** The impact is detected on the entire environment.
By the persistence	**Temporary:** The disruption has a short time of manifestation. **Permanent:** The disruption is undefined in time.
By the resilience of the environment	**Irrecoverable:** The environmental cannot be refurbished to the original state. **Irreversible:** The environment is refurbished by natural means with extreme hardship. **Reversible:** The environment can assimilate the disruption in short term. **Fleeting:** Immediate recovery after the activity has stopped. No corrective measures are needed.

Table 6. Impacts classification. (Own authorship)

Project´s phase	Component	Impact identified	Impact category
Construction phase	Climate	Alteration of local microclimate	Simple, secondary, latent, total, temporary, irreversible.
	Atmosphere	Air quality changes due to machinery	Cumulative, primary, latent, total, temporary, reversible.
		Particle production	Cumulative, primary, immediate, partial, temporary, reversible.
		Noise emissions due to machinery	Synergistic, primary, immediate, partial, temporary, fleeting.
	Soil	Land erosion	Simple, primary, latent, occasional, temporary, irreversible.

Table 7. Impacts classification (Continuation). (Own authorship)

Project´s phase	Component	Impact identified	Impact category
Construction phase	Soil	Soil compaction	Cumulative, primary, immediate, extreme, permanent, irreversible.
		Land pollution	Cumulative, primary, immediate, occasional, permanent, irrecoverable.
		Soil contour disorganization	Simple, primary, immediate, extreme, permanent, irrecoverable.
		Modification of geological formations	Simple, primary, immediate, extreme, permanent, irrevocable
	Water	Pollution of water bodies	Simple, primary, immediate, total, temporary, reversible.
		Decrease in the aquifer recharge capacity	Simple, primary, immediate, partial, temporary, reversible.
	Flora	Loss of vegetable coverage	Simple, secondary, latent, extreme, temporary, reversible
		Loss of individuals from vegetable species	Simple, primary, latent, extreme, temporary, reversible.
	Fauna	Modification of the habitat due to loss of vegetable coverage	Simple, primary, latent, total, permanent, irrevocable.
		Displacement of species due to noise	Simple, primary, latent, extreme, temporary, reversible.
		Loss of individual of animal species	Simple, primary, latent, extreme, temporary, reversible.
	Landscape	Loss of quality of the landscape	Simple, primary, immediate, partial, temporary, reversible.
	Socio-economic	Modification of land use	Simple, primary, latent, partial, temporary, reversible.
		Creation of direct and indirect jobs	Simple, primary, latent, partial, temporary, reversible.
		Demand of services in neighboring towns	Simple, primary, latent, partial, temporary, reversible.

Table 8. Impacts classification (Continuation). (Own authorship)

Project´s phase	Component	Impact identified	Impact category
Operating phase	Atmosphere	Air quality changes due to emissions from the manufacturing process	Cumulative, primary, latent, total, temporary, reversible.
		Noise emissions from equipment	Synergistic, primary, immediate, partial, temporary, fleeting.
	Soil	Land pollution due to management of waste	Cumulative, primary, immediate, occasional, permanent, irrecoverable.
	Flora	Growth of natural vegetation in unused areas	Cumulative, secondary, latent, occasional, temporary, reversible.
	Fauna	Displacement of species due to noise	Simple, primary, latent, extreme, temporary, reversible
	Landscape	Modification of the original landscape	Simple, primary, immediate, partial, temporary, reversible.
	Socio-economic	Generation of direct and indirect jobs	Simple, primary, latent, partial, temporary, reversible.
		Local and regional development	Simple, primary, latent, total, temporary, reversible.
		Services demand for management of waste	Simple, primary, latent, total, temporary, reversible.
Decommissioning phase	Atmosphere	Air quality changes due to machinery	Cumulative, primary, latent, total, temporary, reversible.
		Particle production	Cumulative, primary, immediate, partial, temporary, reversible.
		Noise emissions due to machinery	Synergistic, primary, immediate, partial, temporary, fleeting.
	Soil	Soil refurbishment	Simple, primary, immediate, occasional, temporary, reversible
		Land pollution	Cumulative, primary, immediate, occasional, permanent, irrecoverable.
	Water	Pollution of water bodies	Simple, primary, immediate, total, temporary, reversible.
		Increase in the aquifer recharge capacity	Simple, primary, immediate, partial, temporary, reversible.

Table 9. Impacts classification (Continuation). (Own authorship)

Project´s phase	Component	Impact identified	Impact category
Decommissioning phase	Flora	Growth of vegetable coverage	Cumulative, secondary, latent, occasional, temporary, reversible.
		Flora refurbishment with corrective measures	Cumulative, secondary, latent, occasional, temporary, reversible.
	Fauna	Reincorporation of individuals of the local fauna species.	Simple, primary, immediate, partial, temporary, reversible.
	Landscape	Loss of quality of the landscape due to machinery	Simple, primary, immediate, partial, temporary, reversible.
		Improvement of the landscape quality of the area	Simple, primary, immediate, partial, temporary, reversible.
	Socio-economic	Modification of land use	Simple, primary, latent, partial, temporary, reversible.
		Creation of direct and indirect jobs	Simple, primary, latent, partial, temporary, reversible.
		Demand of services in neighboring towns	Simple, primary, latent, partial, temporary, reversible.

1.4 Alternatives analysis

The analysis of different alternatives for this project has been made in Document I. Descriptive report in section 7 (Study of alternatives). Environmental aspects were considered during the selection process of the alternative as indicated in the table 8 of the document.

1.5 Environmental impacts assessment

Once the environmental impacts generated by this project are known and classified, they should be evaluated. There are different methodologies for impacts identification and assessment in order to determine which physical, chemical, biological or socio-economic variables have effect since the beginning to the decommissioning phase of the project.

The chosen methodology has to adjust to the project´s requirements. For the selection process, the following points has been considered:

- The current legislation, which determines the environmental impact assessment study precision and content.
- The project´s type, magnitudes and complexity.
- The main objective for completion of the environmental impact assessment.
- The different project phases, which must be evaluated and qualified.
- Data requirements for the methodology application.
- The building of relationships between economic costs and expected impacts.
- Results independency, although the evaluators have their subjective perception. [26]

Furthermore, a project impact assessment can be qualitative or quantitative depending of the project level definition. A qualitative impact assessment can be esteemed acceptable for initial stages of any project. The poly (lactic acid) production facility design is considered to have a project definition lower than 40%. For this reason, a qualitative assessment is acceptable. Among the impact assessment methodologies highlights: Ad hoc methodologies, Leopold methodology, cartographer methods, checklists, flow charts, networks, Batelle method, etc. The most used methods are Leopold and Batelle methods. [27]

1.5.1 Impact assessment

A Leopold matrix methodology has been used for this project impacts identification and assessment. It is a matrix structure method which settle a cause-effect relationship between the project´s activities and the environmental impacts affecting it. Both, activities and environmental impacts are introduced in a fourfold table. Environmental impacts influenced by the project´s actions are located vertically while the listed programme actions with effects over the environmental aspects, horizontally.

There are a total of 100 possible programme actions in a simple Leopold matrix and a total of 88 environmental characteristics placed in the vertical axis. Then, 8,800 interactions are produced in the matrix. However, only a few activities produce important effects and the matrix can be considerably simplified.

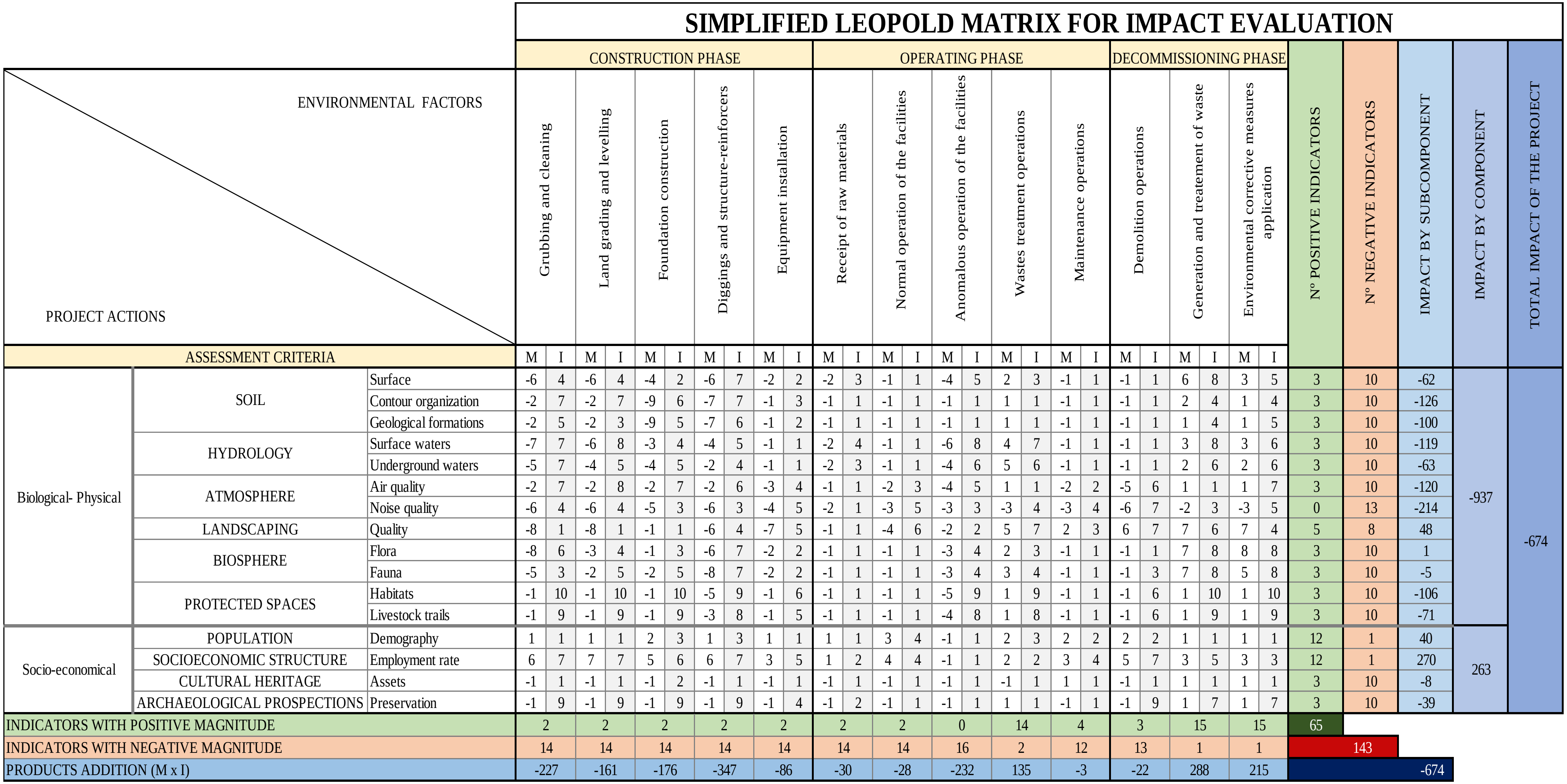
This method helps to determine the interaction between activities and impacts with two selected aspects: the impact magnitude and importance.

The magnitude has extensive values and is outline numerically by a range of 1-10 being 10 the greatest magnitude and 1 the minimum magnitude. A sign + or – can be added for positive and unfavorable effects. The importance is related to the significance of the effect and is defined in a range 1-10, just like the magnitude.

Table 10. Magnitude and importance scale for the Leopold matrix. [28]

Impacts valuation	Magnitude scale (±)1-10	Importance scale 1-10
No impact	1	1
Low impact	2-4	2-4
Medium impact	5-6	5-6
High impact	7-10	7-10

This method allows for a viewing of the cause-effect relationships, for a qualitative assessment and a subjective numerical assessment which indicates the relative significance of impacts at the same time the project is compared with other similar projects. However, the method also has disadvantages. It has a very subjective assessment which strongly depends on the evaluator and static assessment, because it does not change over time and there is not distinction between short and long-term. The Leopold matrix is shown in figure 9.



SIMPLIFIED LEOPOLD MATRIX FOR IMPACT EVALUATION

ENVIRONMENTAL FACTORS / PROJECT ACTIONS			CONSTRUCTION PHASE										OPERATING PHASE										DECOMMISSIONING PHASE						N° POSITIVE INDICATORS	N° NEGATIVE INDICATORS	IMPACT BY SUBCOMPONENT	IMPACT BY COMPONENT	TOTAL IMPACT OF THE PROJECT
			Grubbing and cleaning		Land grading and levelling		Foundation construction		Diggings and structure-reinforcers		Equipment installation		Receipt of raw materials		Normal operation of the facilities		Anomalous operation of the facilities		Wastes treatment operations		Maintenance operations		Demolition operations		Generation and treatement of waste		Environmental corrective measures application						
ASSESSMENT CRITERIA			M	I	M	I	M	I	M	I	M	I	M	I	M	I	M	I	M	I	M	I	M	I	M	I	M	I					
Biological- Physical	SOIL	Surface	-6	4	-6	4	-4	2	-6	7	-2	2	-2	3	-1	1	-4	5	2	3	-1	1	-1	1	6	8	3	5	3	10	-62	-937	-674
		Contour organization	-2	7	-2	7	-9	6	-7	7	-1	3	-1	1	-1	1	-1	1	1	1	-1	1	-1	1	2	4	1	4	3	10	-126		
		Geological formations	-2	5	-2	3	-9	5	-7	6	-1	2	-1	1	-1	1	-1	1	1	1	-1	1	-1	1	1	4	1	5	3	10	-100		
	HYDROLOGY	Surface waters	-7	7	-6	8	-3	4	-4	5	-1	1	-2	4	-1	1	-6	8	4	7	-1	1	-1	1	3	8	3	6	3	10	-119		
		Underground waters	-5	7	-4	5	-4	5	-2	4	-1	1	-2	3	-1	1	-4	6	5	6	-1	1	-1	1	2	6	2	6	3	10	-63		
	ATMOSPHERE	Air quality	-2	7	-2	8	-2	7	-2	6	-3	4	-1	1	-2	3	-4	5	1	1	-2	2	-5	6	1	1	1	7	3	10	-120		
		Noise quality	-6	4	-6	4	-5	3	-6	3	-4	5	-2	1	-3	5	-3	3	-3	4	-3	4	-6	7	-2	3	-3	5	0	13	-214		
	LANDSCAPING	Quality	-8	1	-8	1	-1	1	-6	4	-7	5	-1	1	-4	6	-2	2	5	7	2	3	6	7	7	6	7	4	5	8	48		
	BIOSPHERE	Flora	-8	6	-3	4	-1	3	-6	7	-2	2	-1	1	-1	1	-3	4	2	3	-1	1	-1	1	7	8	8	8	3	10	1		
		Fauna	-5	3	-2	5	-2	5	-8	7	-2	2	-1	1	-1	1	-3	4	3	4	-1	1	-1	3	7	8	5	8	3	10	-5		
	PROTECTED SPACES	Habitats	-1	10	-1	10	-1	10	-5	9	-1	6	-1	1	-1	1	-5	9	1	9	-1	1	-1	6	1	10	1	10	3	10	-106		
		Livestock trails	-1	9	-1	9	-1	9	-3	8	-1	5	-1	1	-1	1	-4	8	1	8	-1	1	-1	6	1	9	1	9	3	10	-71		
Socio-economical	POPULATION	Demography	1	1	1	1	2	3	1	3	1	1	1	1	3	4	-1	1	2	3	2	2	2	2	1	1	1	1	12	1	40	263	
	SOCIOECONOMIC STRUCTURE	Employment rate	6	7	7	7	5	6	6	7	3	5	1	2	4	4	-1	1	2	2	3	4	5	7	3	5	3	3	12	1	270		
	CULTURAL HERITAGE	Assets	-1	1	-1	1	-1	2	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	1	-1	1	1	1	1	1	3	10	-8		
	ARCHAEOLOGICAL PROSPECTIONS	Preservation	-1	9	-1	9	-1	9	-1	9	-1	4	-1	2	-1	1	-1	1	1	1	-1	1	-1	9	1	7	1	7	3	10	-39		
INDICATORS WITH POSITIVE MAGNITUDE			2		2		2		2		2		2		2		0		14		4		3		15		15		65				
INDICATORS WITH NEGATIVE MAGNITUDE			14		14		14		14		14		14		14		16		2		12		13		1		1		143				
PRODUCTS ADDITION (M x I)			-227		-161		-176		-347		-86		-30		-28		-232		135		-3		-22		288		215		-674				

Figure 9. Simplified Leopold Matrix. (Own authorship)

1.6 Environmental protective and corrective measures

The corrective measures allow for the negative effect's reduction, elimination and compensation during a projects execution and protective measures allow for the current environment preservation. Different protective and corrective measures are explained below for the different project phases.

1.6.1 Construction phase

1.6.1.1 Preventive measures

1. Protective measures with regard to the soil:

- The existing road network should be used as much as possible and should be kept in good conditions to prevent the construction of new roads, and avoid the use of a new land. Surface drainage in the roads improved the maintenance operations and avoid the water trails onset.
- The site´s preparation must be done in such way that the wastes production and land movements are minimal. The generated wastes must be removed properly.
- Maintenance and cleaning operations for the construction machinery must not be carried out in the construction site and the machinery must be regularly reviewed, the lubricating oils and fuels leaks can be prevented.
- The fertile soil layer must be taken away and store in good conditions in order to be used in land rehabilitation projects.

2. Protective measures with regard to the atmosphere

- An appropriate machinery maintenance should be done, so the atmospheric emissions are being reduced. The machinery used in the construction works should be environmentally friendly from the current technology point of view and must meet with the noise limits emissions to reduce acoustic pollution.
- Extreme dust production must be reduced during loading and unloading operations.

3. Protective measures with regard to the waters

- Marjal dels Moros humid zone is close to the construction site area. For this reason, the water should not be muddy and the wastes materials should not be deposit on the margins of the humid protected area.

4. Protective measure with regard to the flora

- Previously to the commencement of works, a flora study should be done in order to identify threaten species in the area. Moreover, more soil surface than the indispensable should not be cleared.
- The number of areas where materials can be stored should be minimal and must be devoid of vegetation.
- The construction machinery transit area must be properly signposted in order to reduce destruction of vegetation and soil compaction.
- Minimization of the number of activities producing dust to protect the flora.

5. Protective measures with regard to the fauna

- Control of the emissions and activities having a negative impact on the wildlife must be done. Disturbances caused by undesirable noise, dust, machinery and staff movements must also be controlled.

6. Protective measures with regard to the socio-economic environment

- The construction site must be well signposted.
- The building works must be done as soon as possible and during working hours to minimize discomforts to the population, including the increase in the sound level.
- Cause damage to other existing infrastructures must be avoided.
- Road transports must be done in times of the day with a lowest traffic density. Routing and timetables should be chosen to minimize the traffic disturbances, in particular for special transportation.
- The construction process inert materials must be stack for their disposal and treatment. Urban wastes generated by the staff must also be collected and stored.

7. Protective measures with regard to the heritage

- Land movements must be overseeing by an archeologist. The goal is the damage prevention to heritage features not yet discovered.

8. Protective measures with regard to the landscape

- The unrestrained dumps emergence must be control in order to avoid visual impacts.

- Embankments and fills must be built according to their general rules.
- The construction machinery must be found in perfect state, especially with an adequate condition of the paint.

1.6.1.2 Corrective measures

Some corrective measures taken during and after the construction phase completion are:

- Additional lands for construction works should be rehabilitated, the land is restored to its original state.
- Leftover materials should be removed and treated properly. These materials must be managed according to the Royal Decree 105/2008 of 1 February which regulates the production and management of construction and demolition.
- Structures and roads access which sustained damages during the construction phase must be refurbished.
- The land affected during the construction works must be restored and the damage areas should suffer a replanting process.

1.6.2 Operating phase

Many environmental impacts can be reduced with an appropriate facility´s design if they are included intrinsically. To this is added a continuous monitoring of the facilities with and adequate maintenance during its service life (throughout its period of operation). The lifetime of an industrial facility is variable. In general, the facility can have between 15-30 years of operation time, which is when the equipment become obsolete. However, there are many facilities lasting more than the previously indicated period and the technology evolves very fast. New technologies improving the environmental impacts are continuously being discovered and installed in the facilities. Some specific corrective measures are explained below.

1. Corrective measures in regard to the atmosphere: Process equipment suppling atmospheric emissions must be regularly under maintenance in order to avoid effectiveness decreasing and replacements by obsolescence. Other equipment must also be examined to prevent small leaks of chemical substances in vapor or liquid state ensuring compliance of the emission limits according to regulations.

   Take necessary measures is important when it comes to reduce noises and vibrations to the outside of the facility. Some of these measures can be, for example, the enclosure of noisy activities, using of isolation system and silencers for equipment, processes soundproofing, and equipment with movable parts inspections …

2. Corrective measures in regard to the waters: Liquid effluents must be treated in compliance with dumping limits of industrial waters indicated in the current legislation.
3. Corrective measures in regard to the soil: Wastes produced during the facilities operation must be delivered to an authorized residues disposal manager in order to segregate and treat each type of waste. The storage area for these wastes must be waterproofed, have containment measures for possible spills and have a good maintenance condition of the vessels with wastes.

As more general measures a training to improve awareness among workers about environmental topics can be carried out.

1.6.3 Decommissioning phase

In the decommissioning phase the corrective measures are related to the land, which has been occupy by the facility during the operating phase. There must be a vegetation, landscape and other cultural aspects restore. Replanting of the area with sowing and planting of indigenous species helps the integration with the natural environment. Besides, the species selection has been made according to weather and soil characteristics. The colors of the environment must fit with the species chosen in order not to change the landscape and allow for a homogenous mixing. [29]

1.7 Environmental Monitoring and Management Plan

1.7.1 General considerations

The Environmental Monitoring and Management Plan ensures the verification and analysis of the instructions, corrective and protective measures described in previous sections of this environmental study. It also assesses the project impact on the environmental components (both biological-physical and socio-economic). This Plan will focus on the monitoring during the construction phase and the management during the operating phase. It is targeted to the contractor, the construction manager and to the competent environmental body because it encompasses from the construction works beginning to the facilities decommissioning.

The Plan objectives are:

- In the construction phase: detection and correction of deviations, monitoring of the environmental measures correct execution, determination of measures modification or new measures addition and supervision of the environmental components.
- In the operating phase: Ensure the verification of the correct evolution of the previous phase, supervise the environment and design of operating mechanisms.

1.7.2 Environmental Monitoring and Management Plan implementation

Necessary material must be prepared in order to carry out the Environmental Monitoring and Management Plan. The material preparation actions include calibration of measuring equipment, expendable material purchase and software acquisition for data storage and development of registries. Once the material is ready, data collection, storage and classification should be done. The information gathered is analyzed and assessed taken into account possible sources of mistakes. Corrective and protective measures must be considered during the data assessment because they could not be enough. In that case, their modification is mandatory. Accordingly, the environmental monitoring and Management Plan must suffer a progressive improvement.

1.7.3 Preparation of documentation

As the Environmental Monitoring and Management Plan evolves, a series of guidance documents are prepared.

- Material assets file: This document collects all the information for the materials used during the Plan development. The devises guarantee and technical information, such as calibrations, are included.
- Environmental Monitoring Diary: Document in where dairy information is gathered. General comments, incidents, protective and corrective measures, level of compliance, etc. are recorded in this dairy. It can be subject to inspections required by the competent environmental authorities and will be submitted to those once the construction works are completed.
- Periodic summary reports: Written comments, results, conclusions and guidelines are incorporate to this document. It has a minimum monthly frequency during the construction phase and an annual frequency in the operating phase.
- Corrective measures annual report: The document shows the effectiveness and the degree of implementation of corrective measures. An annual report for corrective measures is elaborated which also includes new suggestions when the measures are insufficient, new environmental impacts are detected or technological progress require so. [30]

1.7.4 Follow-up of the Environmental Monitoring and Management Plan

The project follow-ups are introduced in this section for each of the project´s phases.

1.7.4.1 Construction phase

The “Manual on Good Environmental Practices at Work” must be defined by the contractor and is included during this project´s phase with a route plan and accesses to the area. This manual will be approved by the work´s manager and will be available for the staff. The content includes among other things: land movements, wastes control, forbidden actions, good practices for machinery driving, practices for impact reduction in regard to the flora and wildlife and establishment of a penalty regime.

The “Manual on Good Environmental Practices at Work” is elaborated for a monitoring and control of the construction work activities which may affect the environment. Besides, the activities must be performed employing the best available technologies.

Some activities for the environmental monitoring and management are:

- Territorial demarcation of the area of operation.
- Preparation of guidelines for vehicles in order to protect the atmosphere.
- Elaboration of control and protective measures for the soil, the surface waters, the biotic environment, the archeology, the landscape, etc. (preventive measures has been explained in the section 1.6 of this environmental study).

Reports must be submitted to the competent environmental body in case a special situation may put in danger or deteriorate an environmental aspect.

An environmental monitoring has to be made during the construction phase. The follow-up will be made with a weekly visit. An act of visitation and a monthly follow-up report will be prepared. Incidents, checks over environmental components, corrective measures effectiveness and the results of applying an environmental monitoring plan are some issues added to this documents. Some monitoring activities are included from table 11 to 18.

Table 11. Monitoring and control of the air quality. [31]

Objective	Check the minimum impact of dust and particles clouds.
Indicator	Airborne dust and suspended particles in the vegetation.
Monitoring	Monthly, except during summer periods and with strong winds. In that case, the monitoring should be done weekly.
Analysis	Visual inspection. Identification of dust by the Works management.
Measures	Wetting dusty surfaces.

Table 12. Monitoring and control of noises and vibrations. [31]

Objective	Check the machinery correct conditions.
Indicator	Acoustic pollution level increment.
Monitoring	Annually and a previous control to the Works beginning.
Analysis	Permissible values are exceeded.
Measures	Machine downtime until repaired.

Table 13. Monitoring and control of the waters quality. [31]

Objective	Maintaining quality of the closest water sources during the construction Works.
Indicator	Negative conditions have been detected in the water´s quality.
Monitoring	Performing two water analysis during the Works. In case of results fluctuation, the analysis can be performed with higher frequency.
Analysis	Analysis methodology according to Royal Decree 1514/2009 of 2 October related to underground waters and the Royal Decree 817/2015 related to the surface waters monitoring.
Measures	Treatment, land movement restrictions, barriers, etc.

Table 14. Monitoring and control of the soil. [31]

Objective	Monitoring of the soil characteristics and the erosive phenomena.
Indicator	Visual inspections of the construction Works area.
Monitoring	Biannual check for the auxiliary areas implementation and monthly for labors on the ground. Four annual inspections for erosion, in special after strong rains.
Analysis	The soil gradient, the compactness level and the topsoil thickness (in where the pH, the organic matter and the grading are analyzed.
Measures	Corrective measures when the permissible values are exceeded and affected areas recovery.

Table 15. Monitoring and control of the vegetation. [31]

Objective	Protection of remarkable species and restoration of topsoil.
Indicator	Affected areas and damages in the topsoil have been detected.
Monitoring	Vegetable species controls are done at the Works beginning and there are quarterly inspections with an increasing frequency in relation to the possible affection. Withdrawal topsoil control is performed at the works start and land warehousing, biannually. The sowing will have a monthly control.
Analysis	To conduct regularly floristic inventories, check of the soil thickness, topsoil analysis and soil transplantation control and quality analysis.
Measures	Topsoil damages restoring.

Table 16. Monitoring and control of the wildlife. [31]

Objective	To ensure the minimum impact in the habitats.
Indicator	The wildlife populations located in the surroundings have diminished.
Monitoring	Initial analysis at the Works beginning and, after that, a biannual analysis is performed. One of the analysis must matched with the reproductive period.
Analysis	Register species analysis and threaten analysis species.
Measures	Temporary restrictions for certain areas during the construction works. Some wildlife individuals belonging to a threaten specie may be relocated to some more appropriate habitats.

Table 17. Monitoring and control of the cultural heritage. [31]

Objective	Provide protection to buildings of historic and architectonic.
Indicator	Damages in buildings of cultural interest have been detected.
Monitoring	Previous inspections to the Works starting. Biannual visits for buildings of cultural interest and a quarterly control for archaeological sites.
Analysis	Visual analysis.
Measures	Communication of damages to the competent environmental body and restoration of the damages produced.

Table 18. Monitoring and control of the landscape. [31]

Objective	Minimize the visual impacts of the construction Works.
Indicator	Elevated visual impact of buildings with high height or dimensions.
Monitoring	Biannual visits.
Analysis	Visual inspections.
Measures	Dismantling of elements having a negative impact in the landscape or his viewing.

1.7.4.2 Operating phase

The first years of the operating phase require a high monitoring and control in agreement with the Environmental Monitoring and Management Plan. This is partly due to:

- The corrective and protective measures effectiveness applied during the construction phase is checked. The analysis includes necessary control for all those aspects, such as the noise level, which require the operation condition of the facilities.
- Maintenance and preservation labors are verified.
- Determination of residual impacts in agreement with the corrective and protective measures effectiveness.
- Determination of new impacts.

The monitoring proceeding over the environmental resources is:

- Monitoring of the atmospheric pollution levels. The immission and emission levels must be determined. The emission levels are measured with “in situ” devises and specific techniques.
- Monitoring of the noise levels produced with measurements of the noise emitted and the acoustic protection effectiveness must be analyzed. This control periodicity is quarterly during the first operating year and the control frequency will reduce over

the time when the results indicates the subsequent fulfillment with objectives and legislation.

- Monitoring of the water quality with the pH, temperature, turbidity and color, conductivity, suspended solids, dissolved oxygen, oxygen biological demand, organic carbonate, nitrates, sulfates, chlorides, etc. measurements.
- Monitoring of the wildlife. The facilities installation increases the noise, brightness and pollution in the area.
- Monitoring of the waste and treatment generation.

1.8 Conclusions

This environmental impact assessment report introduces an environmental inventory. The impacts originated from the construction, execution and decommissioning of the polylactic acid production facility were analyzed for each of the items of the named inventory. Finally, protective and corrective measures were proposed.

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DOCUMENT V

Budget

Index

1. Introduction

Document IV, named as budget, introduces a prospective estimation related to the costs of the Work, expenses and incomes of this project. A cost budget can be set taking as basis a cost estimation. The purposes of a cost estimation have to do with an affordability evaluation and necessary calculations required for funding or investment determination, which is expected to be expend in a properly execution of the project.

Cost estimations can also provide information about trade studies, independent reviews, baseline changes and the scheduling of building programs. Its importance lies on the main objectives of the project (which is mainly to make profits).

The cost estimation integrity of a project can be specified with an appropriate cost estimating methodology. Therefore, and summarizing, the cost estimating background is developed by: defining the scope of the project and determining the estimation accuracy, taking into account the risks related to the considered estimation, a classification system of cost estimating and the methodology used.

2. Scope of the project and classification system of cost estimating

2.1 Scope of the project

A project can be defined according to its maturity level, which is linked to the percentage of design completion of the deliverable documents, drawings and plans. This percentage is associated to the estimate class for a cost determination. A class estimation is mainly subjective, although some information, like the one shown in table 1, is making the class selection more objective.

The engineering deliverables considered in table 1 are those needed for a project, according to recommended practices of AACE international (Association for the Advance of Cost Engineering). The named organization was the one which defined the “Cost Estimate Classification System” and has established the five class types of cost estimation.

Table 1. Estimate input checklist and Maturity Matrix for the process industries. [1]

	Estimate classification				
General project data	**CLASS 5**	**CLASS 4**	**CLASS 3**	**CLASS 2**	**CLASS 1**
Project Scope Description	General	Preliminary	Defined	Defined	Defined
Plant production/ Facility capacity	Assumed	Preliminary	Defined	Defined	Defined
Plant location	General	Approximate	Specific	Specific	Specific
Soils and Hydrology	None	Preliminary	Defined	Defined	Defined
Integrated Plan Project	None	Preliminary	Defined	Defined	Defined
Project Master Schedule	None	Preliminary	Defined	Defined	Defined
Scalation Strategy	None	Preliminary	Defined	Defined	Defined
Work Breakout Structure	None	Preliminary	Defined	Defined	Defined
Project Code of Accounts	None	Preliminary	Defined	Defined	Defined
Contracting Strategy	Assumed	Assumed	Preliminary	Defined	Defined
Engineering Deliverables					
Block Flow Diagrams (BFDs)	S/P	P/C	C	C	C
Plot Plans		S	P/C	C	C
Process Flow Diagrams (PFDs)		S/P	P/C	C	C
Utility Flow Diagrams (UFDs)		S/P	P/C	C	C
Piping & Instrument Diagrams (P&IDs)		S	P/C	C	C
Heat & Material Balances		S	P/C	C	C
Process Equipment List		S/P	P/C	C	C
Utility Equipment List		S/P	P/C	C	C
Electric One-Line Drawings		S/P	P/C	C	C
Specifications & Datasheets		S	P/C	C	C
General Equipment Arrangement Drawings		S	P/C	C	C
Spare Parts listings			S/P	P	P
Mechanical Discipline Drawings			S	P	P/C
Electric Discipline Drawings			S	P	P/C
Instrumentation/Control System Discipline Drawings			S	P	P/C
Civil/Structural/Site Discipline Drawings			S	P	P/C

None (blank)= Development has not begun; Started (S) = Work of the deliverable has begun; Preliminary (P) =Work of the deliverable is advance; Complete (C) = Work of the deliverable has approved.

2.2 Classification system of cost estimating (cost estimate class)

Cost estimate classifications are found in the Association for Advancement of Cost Engineering International (AACEI): Recommended Practice (RP) No. 17R-97 and RP No. 18R-97.

The selection/identification of the cost estimation class suitable for a specific project level can be made according to some guideline given for the RP No. 17 R-97, in which the different types of cost estimates are described. There are five types or classes of cost estimates which are designated as class 1, 2, 3, 4 and 5. Class 1 is considered to be the highest-level definition of the project while class 5 is considered to be the lowest one. The table 2 illustrates the five-cost estimate classification with some characteristics like the project level definition, the estimation purpose, the estimating method and the expected accuracy range.

Table 2. Classification Matrix needed for cost estimation of a project investment. [2]

Estimation class	Project level definition	Estimation purpose	Estimating Method	Expected accuracy range
Class 5	0-2 %	Research and viability	Capacity factored, parametric models and judgment	4-20
Class 4	1-15 %	Conceptual study and viability	Equipment factored or parametric models	3-12
Class 3	10-40 %	Budget, authorization and control	Semi-detailed unit costs with assembly line items	2-6
Class 2	30-70 %	Control and tender	Detailed unit cost with force detail take-off	1-3
Class 1	50-100 %	Estimation review and tender	Detailed unit cost with force detail take-off	1

Class 1 and 2 estimates used to be prepared by construction contractors because are needed to support construction bids, among other things. Accordingly, classes 1 and 2 are not estimates to be contemplated during the cost estimations of this project.

On the basis of the previously explained (take a look at tables 1 and 2), this project is going to base its economic decisions on estimates associated with class 4 level of project definition.

Consideration must be given to the accuracy range shown in table 2 because similar accuracy ranges may occur between class 5 when a project has good history and data, and class 3 when the project is new.

2.3 Selected cost estimating method

There are two categories of estimating methodologies depending on the project scope, the estimate purpose, the project maturity and availability of cost estimating resources, which are: conceptual and deterministic methodologies.

Conceptual (stochastic or factored) estimating methods are chosen with a low project definition and require significant effort in data-gathering, in historical cost analysis to develop accurate factors, estimating algorithms to support this type of estimation and in methods development before estimate preparation ever begins. This estimating method category is typically used for class 5 and 4, although can also be used with class 3. Moreover, it is characterized by a quick method determination of the cost of projects with a little scope definition.

For a class 5 or class 4 estimate, conceptual estimating methods help to determine if a project might have project financial limits. For class 3 estimate, this kind of methodology estimation is necessary and an additional investment in design or engineering is of vital importance.

Some of the most commonly used methods of conceptual estimating methods are: physical dimensions, end-product units, capacity factor, parametric modeling and various ratio or factor method.

Deterministic estimating methods are required for a higher project definition than conceptual estimating methods. These methods demand a large effort during the preparation of the estimation because the evaluation and quantification of the project scope can take substantial time. Deterministic estimates are prepared for projects classified on class 3 through class 1 estimate and are elaborated for budget authorization, contractor bid tender or cost control during a project execution. [1]

The estimating method which is going to be used for this project will mainly depend on the level of the project definition and the design information on hand, although there are other factors like the amount of time and money available to prepare the estimate.

As previously defined in section 2.2, this project cost estimations can be classified on class 4. This classification becomes the main reason why the estimating method is conceptual. More precisely, the conceptual estimating method to be used is the factor method.

3. Capital costs estimation

The capital cost of a chemical process plant is the funding necessary to design, purchase, build, install and start up the pieces of equipment of a plant required for transforming materials, so as the facilities and the infrastructure.

The capital cost represents the equity investment in a plant in expectation of future benefits. In order to check if a plant will generate enough returns to make the investment worthwhile, a Capital Cost Estimate (CCE) must be proposed. The total capital investment can be separated into fixed-capital investment (to supply necessary manufacturing and plant facilities) and working capital (necessary for the plant operation)

As already mentioned in previous sections, the cost estimating method to be used is the ratio factor method, also named as “equipment factor”. This method can be applied to estimate the cost of processes and chemical plants when the total cost can be estimated from the cost of a primary component which is an important part of the project cost. This estimating methodology can be used with a class 4 estimate according to a project level definition which is around 1 to 15 percent complete. If this method is used to justified the funding or budget of a project then the estimate classification is class 3. An appropriate cost estimate will be made with this methodology for this specific project.

Over time, different methods or equipment factoring have been proposed. Hans Lang was the first person to introduce factors to estimate the cost, but also highlights some others like W.E. Hand and Arthur Miller. Another method to those submitted previously is the one present bellow. Separate costs are generated for each discipline associated with the installation of equipment. For this reason, when preparing an equipment factor estimate, the first step is to estimate the cost for each piece of process equipment. An equipment list is mandatory and equipment sizing should be also verified. At this stage a normal problem found is related with a 100% equipment dimensioning and, according to this, a certain percentage of oversize is needed. So, the equipment purchase costs should be calculated. Once these costs are established, appropriate equipment factors are applied. Moreover, adjustments for equipment size and operating conditions are included if necessary.

The remainder project costs which have not been covered by the equipment factors must be taken into account. Some of them are related to indirect costs and outside battery limits costs.

3.1 Equipment costs estimation

3.1.1 Correcting equipment cost for size

The calculation of a purchased equipment cost can be determined with an estimating capital investment method like sources of equipment prices, methods of adjusting equipment prices for capacity and methods of estimating auxiliary process equipment. Nevertheless, the most accuracy determination of the equipment cost is obtained from fabricators or suppliers. Other option is to look for files of past purchase orders which must be corrected with the current cost index.

In this project, however, there is no data available of prices for the size of the equipment involve. In the light of this event, cost data can be obtained by adjusting equipment prices for capacity (scaling) and is expressed as a power law capacity.

$$C_E = C_B \left(\frac{Q}{Q_B}\right)^M f_M f_P f_T \tag{1}$$

Where,

C_E = Equipment cost with capacity Q.

C_B = Equipment cost base with capacity Q_B.

M = constant depending on equipment type.

f_M = correction factor for materials of construction.

f_P = correction factor for design pressure.

f_T = correction factor for design temperature.

Equipment cost base Q_B, equipment base capacity and constant M for different equipment items are shown in table 3. This table presents data on the basis of January 2000 costs and the CE Index of Equipment has a value of 435.8.

Table 3. Data for cost correlations with a base capacity in several equipment. [3]

Equipment	**Material of construction**	**Capacity measure**	**Base size Q_B**	**Base Cost C_B ($)**	**Size range**	**Cost exponent M**
Agitated reactor	CS	Volume (m^3)	1	1.15×10^4	1-50	0.45
Pressure vessel	SS	Mass (t)	6	9.84×10^4	6-100	0.82
Distillation column (Empty shell)	CS	Mass (t)	8	6.56×10^4	8-300	0.89
Structured packing (5m height)	SS (low grade)	Column diameter (m)	0.5	1.80×10^4	0.5-4.0	1.70
Shell-and-tube heat exchanger	CS	Heat transfer area (m^2)	80	3.28×10^4	80-4000	0.68
Centrifugal pump (Small, including motor)	SS (high grade)	Power (kW)	1	1.97×10^3	1-10	0.35
Centrifugal pump (Large, including motor)	CS	Power (kW)	4	9.84×10^3	4-700	0.55
Storage tank (Small atmospheric)	SS (low grade)	Volume (m^3)	0.1	3.28×10^3	0.1-20	0.57
Storage tank (Large atmospheric)	CS	Volume (m^3)	5	1.15×10^4	5-200	0.53

CS= Steel Carbon; SS (low grade) = low-grade stainless steel, for example type 304; SS (high grade) = high-grade stainless steel, for example, type 306.

Other equation for the determination of a purchased equipment cost is defined in equation 2. The used of equation 1 of 2 depends on the available data for each equipment of the project.

$$C_E = (a + b\, {Q_B}^{M}) f_M f_P f_T \qquad (2)$$

Table 4. Data for cost correlations with a base capacity in several equipment. [4]

Equipment	Capacity measure	Size range	a	b	n
Vertical tube evaporator	Heat transfer area (m^2)	11-640	17000	13500	0.6
Double-pipe	Heat transfer area (m^2)	1-80	500	1100	1
U-tube kettle boiler	Heat transfer area (m^2)	10-500	14000	83	1
Floating head shell and tube	Heat transfer area (m^2)	10-1000	11000	115	1
U-tube shell and tube	Heat transfer area (m^2)	10-1000	10000	88	1
Vertical pressure vessel, CS	Mass (kg)	150-69200	-400	230	0.6

Table 4 provides data with basis on 2006 with a cost index CE of 478.6.

The purchased cost of the gear pumps and the extruder is obtained graphically from figures 1 and 2.

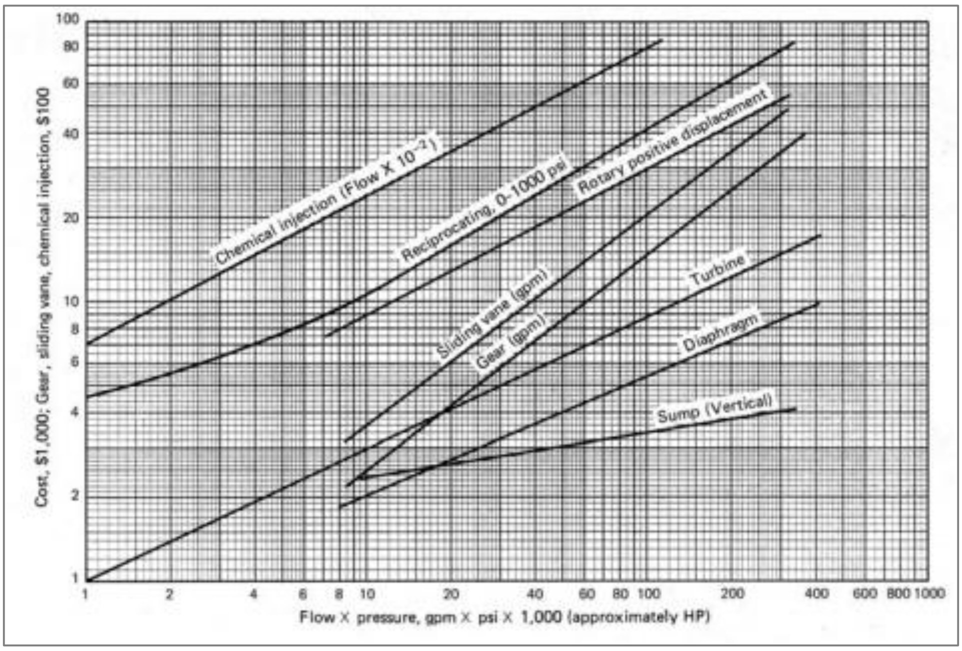

Figure 1. Estimation of the cost of different pumps. [5]

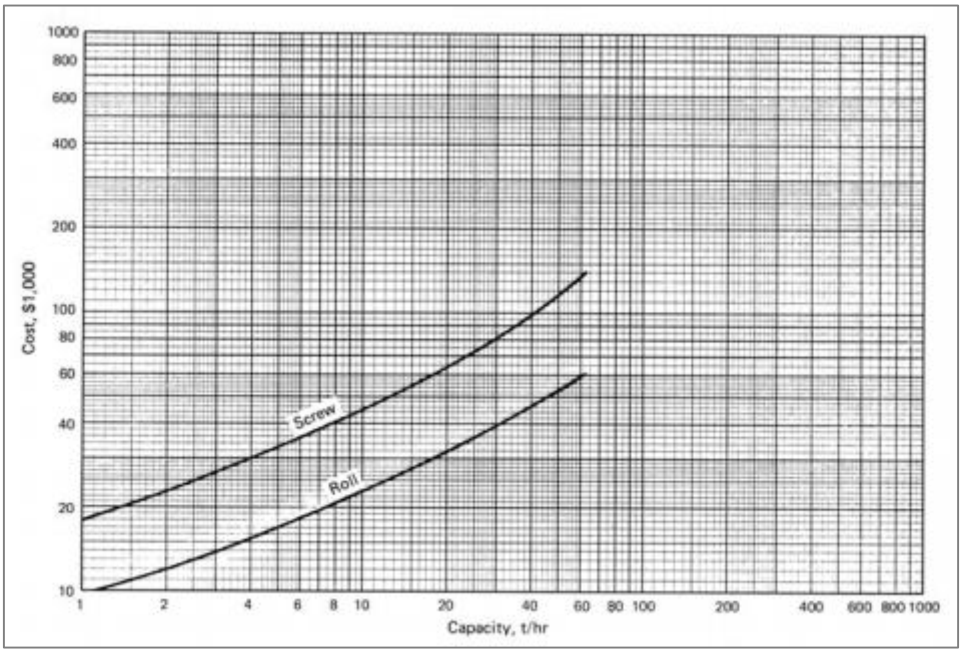

Figure 2. Estimation of the cost of the extruder. [5]

All the information shown in figure 1 and 2 and in table 5 is from year 1974 and the CE index is 320. The information is not very updated but meets with the characteristics of the equipment of the project.

Table 5. Information for the calculation of ejectors. [5]

Equipment	**Material of construction**	**Capacity measure**	**Base size Q_B**	**Base Cost C_B ($)**	**Cost exponent M**
Ejector	Cast iron	lb/h/ (suction vacuum)	1	10000	0.42

3.1.2 Correcting equipment costs for design, temperature, pressure and materials of construction

The costs obtained in the literature contains equipment at base conditions (low temperature and pressure conditions, carbon steel construction and a specific design). The present time of the cost of the equipment is calculated by multiplying the base equation by correction factors, just like was already shown in equation 1 or 2.

Correction factors depend of temperature, pressure, material of construction and type of equipment. All of these correction factors are shown on tables 6, 7 and 8.

Table 6. Cost correction factors for different design pressures [3]

Design pressure (bar absolute)	**Correction factor f_P**
0.01	2.0
0.1	1.3
0.5 to 7	1.0
50	1.5
100	1.9

Table 7. Cost correction factors for different design temperatures. [3]

Design temperature (°C)	**Correction factor f_T**
0-100	1.0
300	1.6
500	2.1

Table 8. Cost correction factor for different materials of construction. [3]

Material	**Correction factor f_M**
Carbon steel	1.0
Aluminum	1.3
Stainless steel (low grades)	2.4
Stainless steel (high grades)	3.4
Hastelloy C	3.6
Monel	4.1
Nickel and Inconel	4.4
Titanium	5.8

3.1.3 Correcting equipment cost for inflation

Data available for calculations related to purchase equipment costs are based on conditions in the past (year 2000 for table 3, for example). However, prices are in constant change. In keeping with this, a method must be used for the updating of this cost data. In order to follow this updating, some cost indexes are going to be used. The calculation of an equivalent cost at present time can be made according to equation 3.

$$Present\ cost = original\ cost\ \left(\frac{index\ value\ at\ present\ time}{index\ value\ at\ time\ original\ cost\ was\ obtained}\right) \tag{3}$$

There are some common indexes like Association of Cost Engineering (ACE) index for erected plant costs, Chemical Engineering (CE) index plant costs, Marshall & Swift (M&S) index for installed equipment and Process Economics International (PEI) index for plant, among others.

There´s something to consider when working with cost indexes. They should only be used to update the type of costs for which they were design. For example, a cost actualization for an equipment can be done with Marshall & Swift (M&S) indexes but not with a Chemical Engineering (CE) index. In addition, cost indexes can only be used to correct a cost in a limit of period of five years because there would be a lack of confidence. The value updated of over five years do not take account of the changes in legislation (especially environmental), health and safety standards, technological advances, …Nevertheless, the information provided in this annex is far more old than 5 years. The lack of more recent information forces the use of this data.

The last cost index known is from 2018 and has a value of 603.1.

3.2 Equipment cost estimation summary

The capital costs of the equipment are collected in tables 9, 10 and 11.

Table 9. Purchased cost of the equipment of the project (Continuation). (Own authorship)

Code	Equipment item	Quantity	Unitary price (€/unit)	Total price (€)
TK-101	Storage tank	1	872,102.60 €	872,102.60 €
E-101	Evaporator	1	597,965.66 €	597,965.66 €
EJ-101	Ejector	1	1,581,396.54 €	1,581,396.54 €
E-102	Condenser	1	43,774.89 €	43,774.89 €
P-102 A/B	Centrifugal pump	2	2,784.40 €	5,568.81 €
V-101	Vapour-Phase Separator	1	331,025.68 €	331,025.68 €
R-201	Reactor	1	6,246,492.04 €	6,246,492.04 €
EJ-201	Ejector	1	124,355.03 €	124,355.03 €
EJ-202	Ejector	1	603,202.23 €	603,202.23 €
P-201 A/B	Gear pump	2	609.19 €	1,218.38 €
V-301	Vapour-Phase Separator	1	78,385.50 €	78,385.50 €
P-301 A/B	Gear pump	2	764.68 €	1,529.36 €
E-301	Heat exchanger	1	75,217.42 €	75,217.42 €
R-301	Reactor	1	72,198.66 €	72,198.66 €
P-302 A/B	Gear pump	2	208.73 €	417.46 €
E-302	Condenser	1	153,552.32 €	153,552.32 €
T-401	Distillation column	1	1,892,619.08 €	1,892,619.08 €
E-401	Condenser	1	83,133.94 €	83,133.94 €

Table 10. Purchased cost of the equipment of the project (Continuation). (Own authorship)

Code	Equipment item	Quantity	Unitary price (€/unit)	Total price (€)
E-402	Reboiler	1	123,092.00 €	123,092.00 €
P-401 A/B	Centrifugal pump	2	4,673.26 €	9,346.53 €
V-401	Vapour-Phase Separator	1	331,025.68 €	331,025.68 €
EJ-401	Ejector	1	262,379.18 €	262,379.18 €
E-403	Condenser	1	34,797.59 €	34,797.59 €
V-402	Vapour-Phase Separator	1	36,044.74 €	36,044.74 €
EJ-402	Ejector	1	103,282.15 €	103,282.15 €
T-402	Distillation column	1	1,388,007.41 €	1,388,007.41 €
E-404	Condenser	1	142,970.79 €	142,970.79 €
E-405	Reboiler	1	221,179.23 €	221,179.23 €
P-402 A/B	Centrifugal pump	2	6,791.55 €	13,583.10 €
V-403	Vapour-Phase Separator	1	20,384.04 €	20,384.04 €
EJ-403	Ejector	1	82,042.41 €	82,042.41 €
V-404	Vapour-Phase Separator	1	12,483.56 €	12,483.56 €
EJ-404	Ejector	1	29,737.72 €	29,737.72 €
E-406	Condenser	1	10,738.94 €	10,738.94 €
E-407	Heat exchanger	1	30,502.76 €	30,502.76 €
P-403 A/B	Centrifugal pump	2	6,791.55 €	13,583.10 €

Table 11. Purchased cost of the equipment of the project (Continuation). (Own authorship)

Code	Equipment item	Quantity	Unitary price (€/unit)	Total price (€)
T-403	Distillation column	1	390,739.35 €	390,739.35 €
E-408	Condenser	1	84,495.50 €	84,495.50 €
E-409	Reboiler	1	112,172.07 €	112,172.07 €
EJ-405	Ejector	1	373,843.14 €	373,843.14 €
EJ-406	Ejector	1	246,494.30 €	246,494.30 €
V-405	Vessel drum	1	12,483.56 €	12,483.56 €
P-404 A/B	Centrifugal pump	2	5,415.11 €	10,830.22 €
P-405 A/B	Centrifugal pump	2	7,045.30 €	14,090.60 €
E-410	Heat exchanger	1	22,348.14 €	22,348.14 €
R-501	Reactor	1	75,483.30 €	75,483.30 €
P-501 A/B	Gear pump	2	69,422.04 €	138,844.07 €
R-502	Reactor	1	322,550.96 €	322,550.96 €
P-502 A/B	Gear pump	2	87,632.32 €	175,264.64 €
X-601	Extruder	1	89,966.39 €	89,966.39 €
E-601	Heat exchanger	1	5,032,375.73 €	5,032,375.73 €
V-602	Vapour-Phase Separator	1	12,483.56 €	12,483.56 €
EJ-601	Ejector	1	81,839.89 €	81,839.89 €
		Total		22,825,641.96 €

4. Part budgets (Capital investment)

The total capital cost of the project is known by the calculation of a series of part budgets accordingly to the Lang factors written in table 14.

Table 12. Lang factors for the approximation of capital investment. [3]

Item	**Type of process**	
	Fluid processing	**Solid processing**
Direct costs		
Equipment delivered cost	1	1
Equipment erection, f_{ER}	0.4	0.5
Piping (installed), f_{PIP}	0.7	0.2
Instrumentation & controls (installed), f_{INST}	0.2	0.1
Electrical (installed), f_{ELEC}	0.1	0.1
Utilities, f_{UTIL}	0.5	0.2
Off-sites, f_{OS}	0.2	0.2
Buildings (including services), f_{BUILD}	0.2	0.3
Site preparation, f_{SP}	0.1	0.1
Total capital cost of installed equipment	3.4	2.7
Indirect costs		
Design, engineering and constructionf_{DEC},	1.0	0.8
Contingency (about 10% of capital costs), f_{CONT}	0.4	0.3
Total fixed capital cost	4.8	3.8
Working capital		
Working capital (15% of total capital cost), f_{WC}	0.7	0.6
Total capital cost, f_I	5.5	4.4

Cost estimations were done in dollars because the data necessary for calculations was found in this monetary units. This project is going to be expressed in euros. Then, the equivalent of one dollar is 0.88 euros.

4.1 Direct costs

4.1.1 Equipment delivered cost

Table 13. Purchase equipment cost. (Own authorship)

Concept	**Description**	**Quantity**	**Price (€)**
Delivered equipment	• Equipment purchase • Transportation • Delivery	Lump sum price	22,825,641.96 €
	Total		22,825,641.96 €

4.1.2 Equipment erection

Table 14. Equipment erection cost. (Own authorship)

Concept	Description	Quantity	Price (€)
Equipment erection	• Structural supports • Insulation • Paint	Lump sum price	9,130,256.79 €
	Total		9,130,256.79 €

4.1.3 Piping

Table 15. Piping cost. (Own authorship)

Concept	Description	Quantity	Price (€)
Piping	• Piping material • Pipe hangers • Fittings •Valves •Insulation-piping	Lump sum price	15,977,949.37 €
	Total		15,977,949.37 €

4.1.4 Instrumentation & Controls

Table 16. Instrumentation and control costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Instrumentation and controls	• Purchase • Installation • Calibration •Computer tie-in	Lump sum price	4,565,128.39 €
	Total		4,565,128.39 €

4.1.5 Electrical

Table 17. Electrical costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Electrical	• Electrical equipment switches • Motors • Conduit, wire and fittings •Feeders •Grounding •Panels	Lump sum price	2,282,564.20 €
	Total		2,282,564.20 €

4.1.6 Utilities

Table 18. Utility costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Utilities	• Fire protection • Environmental controls • Water disposal plant • Water, refrigeration, high pressure steam, medium pressure steam,... • Plant incinerator, wells, river intake, cooling towers,...	Lump sum price	11,412,820.98 €
	Total		11,412,820.98 €

4.1.7 Off-site

Table 19. Offsite costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Off-site	• Auxiliary buildings • Roads and access routes • Communication systems • Products and raw materials storage • Parking area •Collection and distribution systems	Lump sum price	4,565,128.39 €
	Total		4,565,128.39 €

4.1.8 Buildings

Table 20. Building costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Buildings	• Process buildings-substructures, superstructures, platforms, supports, ladders,... • Auxiliary buildings administration • Other buildings for services	Lump sum price	4,565,128.39 €
	Total		4,565,128.39 €

4.1.9 Site preparation

Table 21. Site preparation costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Site preparation	• Land cleaning operation • Excavations and land motions • Garbage collection	Lump sum price	2,282,564.20 €
	Total		2,282,564.20 €

4.1.10 Land

Table 22. Land plot costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Land plot	• Land purchase	Lump sum price	1,601,959.00 €
	Total		1,601,959.00 €

4.2 Indirect costs

4.2.1 Design, engineering and construction

Table 23. Design, engineering and construction costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Design, engineering and construction	• Engineering supervision and inspection • Engineering costs-administrative • Procuring, expediting, reproduction, communications, scale models, consultant fees,…	Lump sum price	22,825,641.96 €
	Total		22,825,641.96 €

4.2.2 Contingency

Table 24. Contingency costs. (Own authorship)

Concept	Description	Quantity	Price (€)
Contingency	• Extra costs in order to face inexpected events (problems, prices changes in raw materials,…)	Lump sum price	9,130,256.79 €
	Total		9,130,256.79 €

4.3 Working capital

Table 25. Working capital. (Own authorship)

Concept	Description	Quantity	Price (€)
Working capital	• Raw materials •Transportation • Initial salaries	Lump sum price	15,977,949.37 €
	Total		15,977,949.37 €

5. Total capital cost

The total capital costs is the addition of all the budget items. The total of the budget is shown:

Table 26. Total budget by items.

Item	Price (€)
Equipment delivered cost	22,825,641.96 €
Equipment erection	9,130,256.79 €
Piping	15,977,949.37 €
Instrumentation & controls	4,565,128.39 €
Electrical	2,282,564.20 €
Utilities	11,412,820.98 €
Off-sites	4,565,128.39 €
Buildings	4,565,128.39 €
Site preparation	2,282,564.20 €
Land plot	1,601,959.00 €
Total of the direct costs	77,607,182.68 €
Design, engineering and construction	22,825,641.96 €
Contingency	9,130,256.79 €
Total of the indirect costs	31,955,898.75 €
Working capital	15,977,949.37 €
Total budget	127,142,989.80 €

The total budget of the construction of a polylactic acid production facility is ONE HUNDRED TWENTY SEVEN MILLION ONE HUNDRED FOURTY TWO THOUSAND NINE HUNDRED AND EITHTY NINE.

Santiago de Compostela, June 2019.

The author,

Sofía Estévez Rivadulla.

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