INTEGRATION OF PRODUCT, PROCESS AND SUPPLY CHAIN DESIGN FOR THE PRODUCTION OF ADDED-VALUE PRODUCTS

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Que la memoria titulada: "Integration of product, process and supply chain design for the production of added-value product", que, para optar al Grado de Doctor en Ingeniería Química con Mención Internacional, presenta **D. Manuel Ralen Taifouris Silva**, ha sido realizada mi dirección dentro del Programa de Doctorado Ciencia y Tecnología Químicas (RD 99/2011) de la Universidad de Salamanca y que, considerando que constituye un trabajo de tesis.

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Su presentación ante la Escuela de Doctorado de la Universidad de Salamanca, mediante el formato de compendio de publicaciones.

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A mis padres y a Carmen

"La ciencia es el motor del progreso humano. Nos permite resolver problemas, innovar y construir un futuro mejor." - Marie Curie

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ABSTRACT

The optimization in the design, production and distribution of value-added products is a key issue in an increasingly competitive market, due to globalization. The most efficient way (economically, environmentally and socially) to design a production process is to consider simultaneously the design of the product, the process and the supply chain, since it allows taking advantage of the synergies of each stage, reducing costs and launching times and increasing the possibilities of customization. This integrated design system is also very useful in waste recovery due to the large number of multi-scale variables that affect recovery. Therefore, this thesis proposes different methodologies for the integrated design of products, processes, and supply chains applied to the production of formulated products and the valorization of different types of waste, from a multi-objective , multiperiod , and multi-scale approach. To find the optimal value of the analyzed variables, different procedures are used, such as reformulations, multistage optimization, as well as the development of linearization and decomposition algorithms. The results showed that, through integrated process, product and supply chain design, it is possible to find a detergent powder formulation that can reduce the environmental impact by up to 40% without reducing the economic benefit by more than 1.5%.Similarly, by applying this integration to animal feed design, meat and crop production can be integrated, using the circular economy of waste. These integrated systems can reduce the environmental impact by up to 62% compared to the decoupled system. The optimal size and location of these facilities was also established. Regarding waste valorization, the integrated design showed that determining the best technology depended on the waste composition, the amount to be treated, and the capital available to invest in its treatment. In the case of coffee valorization, the best treatment process consists of a extraction-filtration system, obtaining a caffeine and pigments. Regarding wine production waste, the most promising process was a hexane and ethanol extraction system, which allows obtaining essential oils, polyphenols and biochar. Finally, this integrated approach is also used to analyze how a country's energy security can be increased through the treatment of its waste, determining that it is possible to cover a demand for natural gas of up to 43%.

RESUMEN

La optimización en el diseño, producción y distribución de productos de valor añadido es una cuestión clave para competir en un mercado global. La forma más eficiente (económica, medioambiental y socialmente) de diseñar un proceso es considerar simultáneamente el diseño del producto, del proceso y de la cadena de suministro, aprovechando las sinergias entre cada etapa, reduciendo costes y tiempos de lanzamiento y aumentando las posibilidades de personalización. Este sistema de diseño integrado también es muy útil en la valorización de residuos debido a las variables multiescala que afectan a la valorización. Por ello, esta tesis propone diferentes metodologías para el diseño integrado de productos, procesos y cadenas de suministro aplicadas a la producción de productos formulados y a la valorización de residuos, desde un enfoque multiobjetivo , multiperiodo y multiescala. Para encontrar el valor óptimo de las variables analizadas, se utilizan diferentes procedimientos, como reformulaciones, optimización multietapa, así como el desarrollo de algoritmos de linealización y descomposición. Los resultados mostraron que, mediante el diseño integrado del proceso, el producto y la cadena de suministro, es posible encontrar una formulación de detergente en polvo que puede reducir el impacto ambiental hasta en un 40 % sin reducir el beneficio económico en más de un 1,5 %. Del mismo modo, aplicando esta integración al diseño de piensos, es posible integrar la producción de carne y de cultivos, utilizando la economía circular de los residuos. Estos sistemas integrados pueden reducir el impacto ambiental hasta un 62 % en comparación con el sistema desacoplado. También se estableció el tamaño y la ubicación óptimos de estas instalaciones. En cuanto a la valorización de residuos, el diseño integrado mostró que la determinación de la mejor tecnología dependía de la composición de los residuos, la cantidad a tratar y el capital disponible para invertir en su tratamiento. En el caso de la valorización del café, el mejor proceso de tratamiento consistió en un sistema de extracción-filtración, obteniéndose cafeína y pigmentos. En cuanto a los residuos de la producción de vino, el proceso más prometedor fue un sistema de extracción con hexano y etanol, que permite obtener aceites esenciales, polifenoles y biocarbón. Por último, este enfoque integrado también se utiliza para analizar cómo se puede aumentar la seguridad energética de un país mediante el tratamiento de sus residuos, determinando que es posible cubrir una demanda de gas natural de hasta el 43 %.

PUBLICATIONS

This thesis is presented as a compendium of publications, where each of the chapters corresponds to a formal manuscript published in a scientific journal, or currently under review. The relation of manuscripts published or under review is detailed below:

Taifouris, M., Martín, M., Martínez, A., & Esquejo, N. (2020). On the effect of the selection of suppliers on the design of formulated products. *Computers & Chemical Engineering*, *141*, 106980.

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Taifouris, M., & Martin, M. (2021). Toward a circular economy approach for integrated intensive livestock and cropping systems. *ACS Sustainable Chemistry & Engineering*, *9*(40), 13471–13479.

Taifouris, M., Martín, M., Martínez, A., & Esquejo, N. (2021). Simultaneous optimization of the design of the product, process, and supply chain for formulated product. *Computers & Chemical Engineering*, *152*, 107384.

Taifouris, M., & Martín, M. (2022). Integrating intensive livestock and cropping systems: Sustainable design and location. *Agricultural Systems*, *203*, 103517.

Taifouris, M., & Martín, M. (2023). Towards energy security by promoting circular economy: A holistic approach. *Applied Energy*, *333*, 120544.

Taifouris, M., El-Halwagi, M., & Martin, M. (Submitted). Evaluation of the economic, environmental and social impact of the valorization of grape pomace from the wine industry. *ACS Sustainable chemistry & Engineering*.

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1

INTRODUCTION

1.1 ADDED-VALUE PRODUCTS

The concept of the added-value product can be applied to any product that, after a series of physical or chemical processing, acquires a higher marketing value than the starting product. In fact, the requirements according to U.S Department of Agriculture (USDA), 2015 for a product to be classified as a added-value product are as follows:

- A change in the physical state or form of the product that allows an increase in its value with respect to the initial product.
- The production of a product in a manner that increases its value.
- The physical segregation of an agricultural commodity or product in a manner that results in the enhancement of the value of that commodity or product (such as an identity-preserved marketing system).

As can be seen, these requirements can be easily extrapolated to waste valorization (Nayak & Bhushan, 2019), which meets the third requirement, or to the production of formulated products (Kontogeorgis et al., 2022), which simultaneously meets requirements 1 and 2.

On the one hand, waste has zero or even negative value (both from an economic and environmental points of view) so any product that can be obtained from it and marketed is considered a added-value product. On the other hand, formulated products are the combination of a series of compounds to produce a complex product designed to meet several requirements simultaneously (Conte & Gani, 2011). This product is not only more complex but also has a higher market value than each product would have separately (Martín & Martínez, 2013).

The production of added-value products is aligned with the achievement of several of the Sustainable Development Goals (Nations, 2022). In 2015, the members of the united nations agreed on 17 goals to make the world fairer, more prosperous, and environmentally friendly. These can be seen in Figure 1.1.

From these goals, waste valorization contributes to goals 12 (responsible consumption and production), 13 (climate action), 15 (life on land), and

Figure 1.1: Sustainable development goals

depending on the product obtained from the waste, it could contribute to goal 7 (affordable and clean energy). Therefore, it could be said that the present thesis would actively contribute to the fulfillment of sustainable development goals.

Next, the different strategies to obtain value from waste valorization and the production of formulated products will be explained in detail, as well as the relevance of the integration of product design, process, and supply chain in this process.

1.2 ADDED-VALUE PRODUCTS FROM WASTE.

Examples of added-value products are all petroleum derivatives, which leads to the design of refineries. However, petroleum is not the only complex feedstock from which a wide variety of products can be obtained, biomass is another example (Tuck et al., 2012). The biorefinery concept was established as a parallel to crude oil processing facilities, where from a feedstock consisting of a mixture of species a portfolio of products is obtained. Similarly, biomass can be processed into a range of valuable products (Chaturvedi et al., 2020).

The need to control CO2 emissions provided the first stimulus for the design of biofuel production facilities, bioethanol, and biodiesel, as substitutes for crude oil-derived gasoline and diesel. They were the main products of the biorefineries. The low-profit margins compared to refineries presented the opportunity to transform these single-product facilities into multi-product facilities through the utilization of the by-products generated, such as distiller's dry grains with solubles or glycerol (Karuppiah et al., 2008; Martín & Grossmann, 2012). These facilities evolved into integrated plants that, using biomass of different types, could self-produce the intermediate products needed for the manufacture of advanced products. An example can be a diesel substitute facility that produces biodiesel and glycerol esters from algae. The i-butene needed to obtain the glycerol esters is obtained from glucose fermentation (De La Cruz et al., 2014), as well as integrated multi-product facilities from lignocellulosic biomass that produce platform chemicals and fuels (Bond et al., 2014).

The use of biomass as a feedstock is experiencing another revolution. Biomass is too valuable to produce energy, fuels, and bulk chemicals. Although the competition between biomass and crude oil for the production of chemicals is unbalanced, due to the large number of steps required to convert the biomass into a useful product, the use of it for the production of chemicals and fuels (Martin & Grossmann, 2013a, 2013b), levulinic acid (Alonso et al., 2013), furfural and either hydroxymethylfurfural (Torres et al., 2010) and dimethyl furfural (Martin & Grossmann, 2016), and diols (Huang et al., 2017), among others, has been investigated. The variety of products that can be obtained from biomass is immense, as can be seen in Figure 1.2 below.

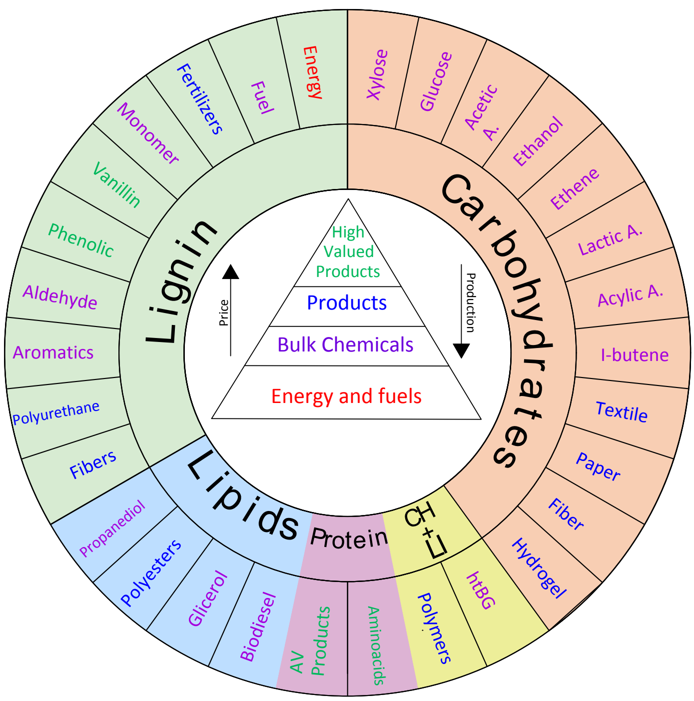

Figure 1.2: Basic, intermediate and final products which can be produced from wastes

The food industry highlights as one of the largest generators of organic waste (Mirabella et al., 2014; Angili et al., 2022). Processes such as the production of orange juice (Criado & Martín, 2020), oil (Guerras et al., 2021), wine (Rodrigues et al., 2022) or coffee (Banu et al., 2020) generate wastes that contain in their composition a set of products with high-added value. These products can be used directly in the food or pharmaceutical industry, as is the case of polyphenols (Brazinha et al., 2015). Others, such as tannins, can be used as pigments in the textile industry (Koh & Hong, 2019) or to produce resins, polymers, and adhesive products (Ping et al, 2010). The production of essential oils (Bustamante et al., 2016), which can be devoted to produce food supplement or cosmetics, are also a common product of waste valorization. Lower value products, such as fertilizers (Mata-Alvarez et al., 2000), biochar, and bio-oil (Williams, 2013), can be obtained as secondary products. All these processes do not only favor the circular economy of the process in the food industry, reducing waste production but also increasing the economic viability of the whole process, reducing energy dependence and water consumption and increasing the sustainability of the process (Slorach et al., 2019). However, the amount of these compounds in these wastes is very variable (Rodrigues et al., 2022), and in some cases, very small. Therefore, it is necessary to correctly analyze their composition when selecting, optimizing, and designing the treatment process. Normally, the high added-value products that can be produced from waste usually represent a very low percentage compared to the amount of fuels or energy, as shown in Figure 1.1.

1.3 ADDED-VALUE PRODUCTS FROM THE BLENDING OF SIMPLER PRODUCTS

In addition to obtaining value from waste treatment, it is possible to obtain value by mixing, in the appropriate proportions, a series of ingredients of less value than the final product. Such products are called formulated products. This type of product is aimed at simultaneously satisfying several specific needs that could not be met by a single chemical compound. Each of the chemical compounds can be custom designed to meet one or more needs (molecular design (Ng et al., 2015)) or existing chemical compounds can be used. The design of this type of product is complex because it is necessary to analyze not only the physicochemical properties of each compound but also the possible interactions present between the ingredients (Bogdanić & Vidal, 2000). These types of products are especially common in consumer products, such as food, detergents, or cosmetics. The correct release of a detergent or drug, the taste of a food, or the smell of a perfume depends on the proper formulation of their ingredients. The value of these products depends on their formulation and is always greater than that of the individual ingredients. The performance of such products is usually assessed by mapping customer needs through market research using machine learning and big data (Wang et al., 2018).

1.4 INTEGRATION OF PRODUCT AND PROCESS DESIGN.

A formulated product must not only meet the requirements of the target customer but must also be feasible to produce on a large scale from an economic, environmental, and social points of view (Bernardo & Saraiva, 2005; Misener et al., 2010). Therefore, the formulation and its production process must be designed together through the so-called 'blending problems'. Blending problems are widely known in the chemical industry (Symonds, 1956; Arthur & Lawrence, 1980) . A particular case of this type of problem would be pooling problems. The main difference between the two problems is that blending problems do not involve intermediate tanks for product formulation (Visweswaran, 2008). They were first identified in refineries for fuel production and in thermal power plants for the proper blending of coal to avoid or reduce combustion emissions (Shih & Frey, 1995). However, pooling problems quickly extended to other industries, such as agriculture, mining, food manufacturing, and the production of paper, among others (Visweswaran, 2008). The pooling problem has also found applications in the analysis of diverse mixtures, such as polymer blends (Vaidyanathan et al., 1998), refrigerant blends (Churi & Achenie, 1997), repellent lotions (Conte & Gani, 2011) and surfactant design (Mattei et al., 2014), among other substances. The general scheme of a pooling problem can be seen in Figure 1.3.

1.4.1 *Modeling approach for the formulated product and process design*

The mathematical formulation of a pooling problem can be easily generalized (Misener et al., 2010). This type of problem is modeled as an optimization problem where the objective function can be to maximize an economic benefit, minimize a cost or an environmental impact, and which is subject to a series of constraints (Eqs.(1.1)-(1.7)) (Martín & Martínez, 2013). To better understand these constraints, Figure 1.3 can be consulted.

$$A_i^L \leq \sum_{Tx} x_{i,l} + \sum_{T_z} z_{i,l} \leq A_i^U \quad \forall i \tag{1.1}$$

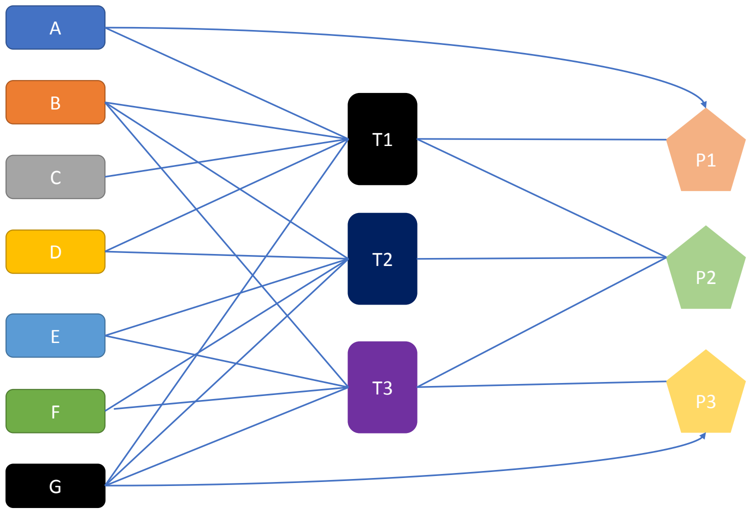

Figure 1.3: Basic scheme of a pooling problem

$$\sum_{Tx} x_{i,l} \leq S_l \quad \forall l \tag{1.2}$$

$$D_j^L \leq \sum_{T_y} y_{l,j} + \sum_{T_z} z_{i,j} \leq D_j^U \quad \forall j \tag{1.3}$$

$$\sum_{T_x} x_{i,l} - \sum_{T_y} y_{l,j} \leq 0 \quad \forall l \tag{1.4}$$

$$\sum_{T_x} C_{i,k} \cdot x_{i,l} - p_{k,l} \sum_{T_y} y_{l,j} \leq 0 \quad \forall l, k \tag{1.5}$$

$$\sum_{T_z} z_{i,j} - \sum_{T_y} p_{k,l} \cdot y_{l,j} \leq P_{j,k}^U \quad \forall l, k \sum_{T_z} z_{i,j} - \sum_{T_y} p_{k,l} \cdot y_{l,j} \geq P_{j,k}^L \quad \forall l, k \tag{1.6}$$

$$\begin{aligned} 0 &\leq x_{i,l} \leq \min\left\{A_i^U, S_l, \sum_{T_y} D_j^U\right\} \quad \forall T_x \\ 0 &\leq y_{l,j} \leq \min\left\{S_l, D_j^U, \sum_{T_x} A_l^U\right\} \quad \forall T_y \\ 0 &\leq z_{i,j} \leq \min\left\{D_j^U, A_l^U\right\} \quad \forall T_z \end{aligned} \tag{1.7}$$

The superindices U and L represent the upper bound and lower bound, while the subindexes 'i','k','j', and 'l' represent the type of raw material, ingredients, products, and mixing pools, respectively. The variables x, y, and z correspond to the material flows from raw material input 'i' to pool 'l', the flows going from intermix pools 'l' to the final product 'j', and the flows going directly from raw material input 'i' to final product 'j', without intermediate mixing, respectively. A_i is the availability of ingredient 'i', D_j is the demand for product 'j' and S_l is the size of the intermediate tanks. $P_{l,k}$ is the composition of ingredient 'k' in pool 'l' and $PQ_{j,k}$ is the final formulation of product j. $C_{i,k}$ is the composition of component 'k' in input stream 'i'.

However, it is important to note that the set of constraints may increase considerably as the set of objectives (economic, environmental, and/or social), the complexity of the process, or the product constraints increase. A generic example of the environmental impact assessment associated with the formulated product is shown in Eq.(1.8).

$$CO2eT = \sum_j \sum_i \sum_k CO2e_k \cdot CC_{i,k} \cdot z_{i,j} + \sum_l \sum_i \sum_k CO2e_k \cdot CC_{i,k} \cdot x_{i,l} \quad (1.8)$$

Where $CO2e_k$ is the carbon footprint of ingredient 'k' (organization, 2017).

Other environmental impact studies simultaneously cover other impact areas, such as LCA and global impacts (Vinodh & Rathod, 2010) .

Some common process constraints can be limits on the operation of the units (Temperature and/or pressure), and the composition of the products or raw materials. The general objective function is shown by Eq.(1.9).

$$\begin{aligned} objval = & \sum_j (\sum_l y_{l,j} + \sum_i z_{i,j}) \cdot priceP_j - \sum_{l,j,loc} Cpool \cdot y_{l,j,loc} \\ & - \sum_i ((\sum_l x_{i,l} + \sum_j z_{i,j}) \cdot priceI_i) \end{aligned} \quad (1.9)$$

From a mathematical standpoint, the salient attribute of these problems is the inclusion of bilinear terms and non-linear, non-convex equations. Consequently, the use of conventional commercial local solvers may not be optimal, as the presence of multiple local optima can hinder their ability to provide the optimal solution or even preclude the generation of any result at all. Thus, the development and continued refinement of global solvers is imperative for effectively addressing these challenges (McCormick, 1976; Wicaksono & Karimi, 2008).

1.4.2 *Integration of product and process design applied to waste valorization*

For optimal waste valorization, it is necessary to evaluate the possible products that can be obtained from the waste composition and their end uses to estimate their value and the final consumer, as well as the physical-chemical processes to obtain these products (Nayak & Bhushan, 2019). This type of study is usually performed at the laboratory level, focusing on the characterization of the raw material and evaluating the physicochemical and biological properties of the products obtained (Angili et al., 2022), so as to select the potential products that could be marketed. However, in some cases, the number of products that can be used is extremely large (Caldeira et al., 2020), but not all of them are viable from an economic, environmental, and social points of view. Therefore, the analysis of the valorization of waste must be coupled with the modeling and optimization of its potential treatment processes. Through techno-economic, environmental, and social analysis (multi-objective optimization) it is established which are the products with the greatest potential to obtain value from a specific waste (Caldeira et al., 2020). Since the composition of the same waste can vary considerably (Rodrigues et al., 2022), it is necessary to perform this type of analysis whenever a new waste recovery line is to be implemented.

In some cases, the composition of the waste will not only determine its treatment process but can also determine whether that waste is valorized or not, depending on the budget constraints available for the construction of valorization plants. Taifouris and Martín, 2018 showed that, depending on the budget available for waste treatment in Castilla y León, one type of waste or another is selected depending on its composition. This not only gives a multi-scale dimension to the problem, but also makes the integration of product and process design of great importance in waste valorization processes.

To systematically evaluate trade-offs and alternatives, superstructures are developed that consider all possible processes, while the amount of raw material sent to each process is a variable of the formulated optimization model. A generic case can be seen in Figure 1.4. Thus, depending on the objectives set, the composition of the waste, the treatment capacity, and the available budget, one process or another and a certain product portfolio will be chosen. These superstructures are the basis of integrated biorefineries that use one or more wastes as feedstock (Umeda et al., 1972). They can be designed as an additional line to a larger process or constitute an independent process in itself oriented to favor circular economy and zero-emission process philosophy. In addition, part of the raw material can be used to produce energy to supply the rest of the process, making it energy self-sustainable.

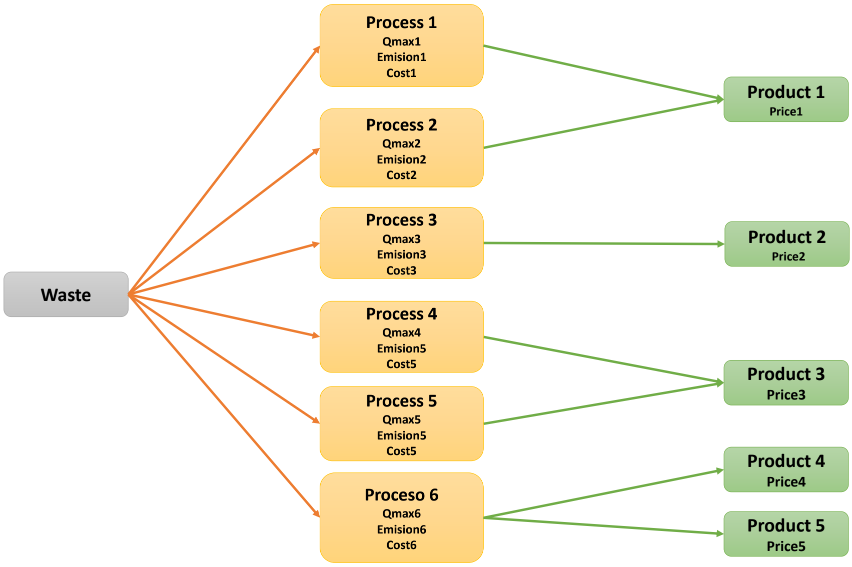

Figure 1.4: Generic superstructure for 5 differents products

In addition to those wastes whose composition is fixed by the processes that produce them, it is also possible to influence the composition of the waste in order to optimize its valorization. This is possible, for example, in the growth of algae (Martin & Grossmann, 2013b), or by adjusting the animal feed to control the composition of the excreted waste (Council, 2000). Different types of waste can also be mixed to find an ideal composition to produce a added-value product. The procedure consists of 3 stages:

- The properties of the product to be obtained are set.
- The composition of the available biomasses is analyzed.
- The proportion of each biomass is adjusted to obtain the desired product.

An example of this procedure can be seen in the work of Hernández et al., 2017. However, for some processes, waste mixtures must be verified from an experimental point of view. For example, in the case of biogas production, the microorganisms responsible for the stages of acidogenesis and methanogenesis are particularly sensitive to many factors, including the amount and quality of the substrate (Chen et al., 2008). These microorganisms can suffer inhibition by excess substrate or by the presence of toxic compounds that are present in some substrates, such as municipal solid waste. Therefore, empirical studies are needed to analyze possible synergies or inhibitory effects between substrates and microorganisms that may increase or decrease the biogas production capacity or the quality of the digestate produced (Lin et al., 2011). This makes the integration of product and process design essential in this type of valorization process. Hence, the resolution of such problems enables the identification of a suitable type of biomass for a given application or the optimization of a specific biomass composition for a particular purpose, thereby facilitating the engineering of a plant to attain the desired outcome.

1.4.2.1 *Modeling of the processes of waste valorization.*

The modeling of the physical and chemical processes involved in the valorization of products can be approached following different strategies depending on the level of detail required, the information available, and the total size of the model. Following the classification proposed by (Martín & Grossmann, 2021), the following methodologies are presented:

Mechanistic models

- Shortcut methods: This method is one of the simplest methods to represent physical systems but also the most basic. They are used when information about the system is scarce or an approximate representation of the physical system to be modeled is desired, for example, for feasibility studies. They are based on a simplified application of first principles, relying mainly on material and energy balances combined with empirical results for the determination of conversions and yields. Thanks to their simplicity, they can be integrated into the design of supply chains and are the best choice when many simple processes are available, among which the best one has to be chosen. However, one of their limitations is the difficulty of modeling complex processes. This type of model is also used in supply chain or process operations.
- Detailed models: These models allow capturing the underlying physics, chemistry, and biology of the systems they model, allowing a better approximation of first principles than in the previous method. These models include thermodynamic and kinetic models (Loeppert et al., 1995; Buzzi-Ferraris & Manenti, 2009), as well as continuity, momentum, and energy equations (Anderson & Wendt, 1995). The mathematical complexity of these models makes their optimization very difficult when the system to be addressed is composed of many equations.

Empirical models

- Rules of thumb: The rule-of-thumb modeling system condenses the knowledge gained from experience into a set of rules that can be applied directly to the design of equipment, processes, and systems. Although these rules can only be applied for very specific cases, they reflect the actual operation of physical systems. These rules are compiled in the works of Couper et al., 2005 and (Hall, 2017)

- Dimensionless analysis: This approach allows the scaling of the systems to be modeled, based on dimensionless relationships that explain physical and chemical phenomena occurring in the system (Szirtes, 2006). Although they are very useful, not only a great deal of experimental work is needed, but also a perfect knowledge of the system to be modeled is necessary to reach and understand these relationships, which can be complicated for novel systems or processes.

- Surrogate models: This type of system modeling allows obtaining simple models, which can be easily integrated into multi-scale optimization models, from rigorous models. The idea is to carry out a rigorous simulation (through mechanistic models or dimensional analysis) of a particular system and build a simplified model from it (Queipo et al., 2005). These models can be built from polynomial regressions (Montgomery et al., 2021), Kriging models (Quirante et al., 2015), or neural networks, which are capable of, through the data of the rigorous model, capturing the relationship between the variables of interest of the system and transfer these relations to the optimization model (Himmelblau, 2000).

- Experimental correlations: In this type of modeling, the physical and chemical characteristics of the systems are captured by experimentation. For this, it is necessary to correctly set the independent variables that will affect the target-dependent variable, to avoid misinterpretation of the results. This type of modeling is relatively easy to integrate into multiscale models but can only be applied within the limits of experimentation.

Machine Learning-based models

- Factorial design of experiments (DOE): It is often used to study processes that are difficult to model due to the large number of variables involved in the physicochemical principles of the system. These models are obtained by analyzing the response variables of a system as a function of fixed input variables.

- Artificial Neural Networks (ANN): The model imitates the behavior of the human brain to predict a response of a system from a previous training with a known data set of the system. The input signal of each neuron is activated or deactivated using a weighting factor, depending on the training data. The signal resulting from the sum of the signals of each neuron (neural network) is sent to a transfer function to give a result of the dependent variable.

- Kriging modeling: The idea is to interpolate a particular point taking into account the nearest available data in the neighborhood assuming a linear correlation. The contribution of the different data points is related to their proximity. Thus, spatial interpolation estimates the relationship between variables, assigning a weight to each variable as a function of distance.

It is necessary to analyze in each case, which modeling approach is the most appropriate to represent the physicochemical system to be addressed. However, for the design of superstructures, it is common to use a combination of shortcut methods with experimental correlations and surrogate models. This is because, when considering simultaneously, in the same optimization model, many processes, applying rigorous models becomes infectable due to the mathematical complexity of the optimization model. In addition, this type of study based on superstructures is usually a techno-economic feasibility study, which is a stage prior to the rigorous design of the treatment line, so it does not require such high precision as that provided by the rigorous models. The idea is to apply these rigorous models to the design of the process or processes selected by the superstructure.

1.4.2.2 *Integration of product, process, and supply chain design*

Introducing a new product in an increasingly competitive market is a very complicated process that requires a deep understanding of customer needs and the entire market chain, which are becoming increasingly complex (Uhlemann & Reiß, 2010). It is no longer sufficient that there is a demand for the product, but it must be of high quality and at a reasonable price. In addition, due to increased environmental awareness, consumers are looking for environmentally friendly products whose traceability can be guaranteed (Yue et al., 2013). Therefore, integrated product design approaches are becoming very important. Figure 1.5 represents the wide variety of factors that can affect the design of a formulated product.

Simultaneously designing the product, the production process, and the supply chain has the following advantages:

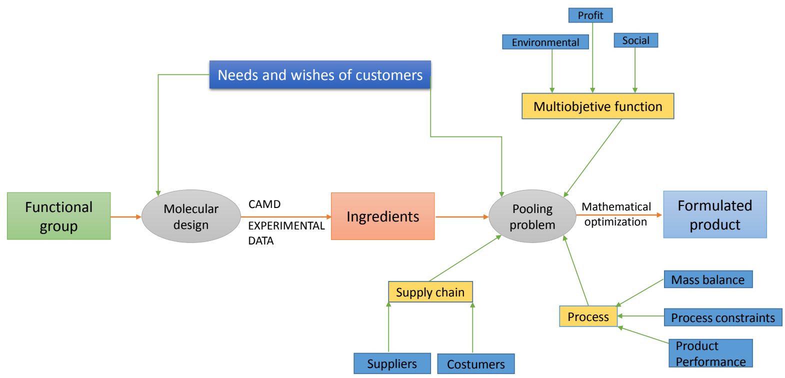

Figure 1.5: Extended design of formulated products.

- It allows discarding product designs whose large-scale production is not economically or environmentally feasible, which reduces time to market and saves on R&D phases by discarding many designs that will not have to be experimentally evaluated.
- It allows for the evaluation of the environmental impact and costs of the whole process, from the conception of the product idea to its delivery to the consumer, being able to identify bottlenecks or designs that balance all objectives, coordinating each phase of development. In addition, it allows the evaluation of the availability of raw materials, and adjusting transportation costs by choosing ingredients that can be purchased locally.
- It allows to adapt the product composition to meet the consumer demands up to the level of customized products, and to reduce delivery times. It also facilitates full product traceability.

Integrated design is particularly important in the case of formulated products since their design depends on their formulation, which can be modified during the production process. Similarly, when designing a newly formulated product (detergents, fertilizers, foods, perfumes, etc.), the set of feasible products to be investigated is broad. Integrated design can act as a screen to substantially reduce the spectrum of possible formulations. The problem begins with the design and/or selection of the ingredients that will be part of the final product. The design of the final product is carried out in a blending process that can be modeled as a pooling problem. According to the concept of integrated product design, the fraction of each ingredient in the final product will be influenced by supply chain characteristics, process constraints, objectives to be met (economic, environmental, and social), and consumer demands. Therefore, all these factors must be integrated into the mathematical model to be used to obtain the optimal product formulation. This approach can be applied both to products that are a mixture of simpler products (in the case of detergents) and to those cases in which a portfolio of products can be obtained from a complex raw material (residues).

In the case of waste, supply chains are simplified to facility location problems, since it is neither cost-effective nor safe to transport waste (Makara & Kowalski, 2018). Typically, waste recovery facilities are installed as an additional unit to the process that generates such waste.

Although there are three stages or levels of the problem, in order to properly assess the synergies between them, it is necessary that all of them are evaluated simultaneously (product, process, and supply chain design (or plant location in the case of waste treatment). Mathematical models to address this type of problem are often difficult to solve. Modeling production processes requires the use of non-linear and non-convex equations (material balances, process constraints, scaling, etc.), as well as bilinear terms. Supply chains also involve decision variables related to the selection of suppliers, locations, customers, etc., which are usually binary variables. When these models reach sizes corresponding to millions of equations and variables, commercial solvers cannot find the optimal values of the variables because the feasible region to be searched is too large and integers (discontinuous problems). The approach to this type of problem (MINLP) will be discussed in Section 1.6.

1.5 MODELING APPROACH OF THE INTEGRATION OF PRODUCT, PROCESS, AND SUPPLY CHAIN DESIGN.

As mentioned in the previous section, only in the case of formulated products, the design of a supply chain and its subsequent integration with the process and product design are considered. For the particular case of waste recovery, the supply chain design is replaced by a facility location problem. Therefore, we proceed to present the general formulation of supply chain integration in integrated process and product design for formulated products (Taifouris & Martin, 2022). First, two continuous variables representing the flow of raw materials to potential facilities ($ccp_{i,sup,loc}$) and another one representing the flow of products to customers ($cv_{j,cost,loc}$) are introduced. The subscripts 'i', 'sup', 'loc', and 'cost' represent the type of raw material, the raw material supplier, the chosen location, and the customer, respectively.

The relationship between $ccp_{i,sup,loc}$ and the internal flows of the production plants ($x_{i,l,loc}$,$z_{i,j,loc}$) is shown by Eq.(1.10).

$$\sum_{sup} ccp_{i,sup,loc} = \sum_{l} x_{i,l,loc} + \sum_{j} z_{i,j,loc} \tag{1.10}$$

The sum of the production of all plants must be less than the maximum demand and greater than the minimum demand, Eq.(1.11) and Eq.(1.12).

$$\sum_{loc} cv_{j,cust,loc} \geq D^{L}_{j,cust} \tag{1.11}$$

$$\sum_{loc} cv_{j,cust,loc} \leq D^{U}_{j,cust} \tag{1.12}$$

The formulation of products, as well as the selection of customers and suppliers, can be chosen through the continuous variables presented above ($ccp_{i,sup,loc}$ and $cv_{j,cost,loc}$), while the use of binary variables is only necessary to consider the fixed costs associated with the construction and operation of manufacturing plants. These variables can be set from the vector of finished products (Eq.(1.13)) since only constructed plants can manufacture products.

$$\sum_{cust} cv_{j,cust,loc} - bi\left(loc\right) \cdot U \leq 0 \tag{1.13}$$

Where U is a large enough value.

In this type of problem, it is necessary to consider the transportation costs, both raw materials (Supcst) and finished products (Delcst). Their calculation is shown by equations Eqs. (1.14) and (1.15).

$$Delcst = \frac{d \cdot Transcst}{Q_{truck}} \cdot Pamt \tag{1.14}$$

$$Supcst = \frac{d \cdot Transcst}{Q_{truck}} \cdot Iamt \tag{1.15}$$

Where d is the distance between the factory and the supplier (or customer), Transcst is the transportation cost, Qtruck is the loading capacity of the truck, Pams is the amount of product and Iamt is the amount of ingredients.

The income generated by the sale of the products (Income) is estimated by Eq. (1.16).

$$Income = \sum_{j,cust,loc} cv_{j,cust,loc} \cdot price_j \tag{1.16}$$

And therefore, the objective function based on the economic performance of all facilities is shown by Eq.(1.17).

$$\begin{aligned} objval = &\sum_{j,loc,cli} cv_{j,loc,cli} \cdot priceP_j - \sum_{l,j,loc} Cpool \cdot yl,j,loc - \sum_{i,sup,loc} ccp_{i,sup,loc} \\ &\cdot priceI_{i,sup,loc} - DeliveryCost - Supplytransportcost - \sum_{loc} bi_{loc} \cdot Fixcosts_{loc} \end{aligned} \tag{1.17}$$

In the case of the facility location problem, the formulation is similar but without the corresponding vector $ccp_{i,sup,loc}$ since the waste, which is the raw material of the waste recovery facilities, is generated in the facilities themselves.

1.6 OPTIMIZATION OF INTEGRATED PRODUCT, PROCESS AND SUPPLY CHAIN DESIGN

As discussed in the previous section, there are many ways to model a physicochemical system. However, its optimization depends not only on the procedure used to model it, but also on the size of the system, its complexity, and the type of variables it uses. The various mathematical optimization formulations that can be used to find one or more optimal solutions to this type of design problem are presented below (Floudas, 1995; Grossmann, 2021).

Linear programing (LP)

This type of optimization consists of the minimization or maximization of a linear objective function, where the rest of the constraints are also linear (Dantzig, 1963). Its mathematical expression is shown in Eq.(1.18).

$$\begin{aligned} \min \quad & Z = c^T x \\ \text{s.t.} \quad & Ax = b \\ & x \geq 0 \end{aligned} \tag{1.18}$$

Where A is a matrix of dimension m x n, c is an n-vector of weighting, x is an n-vector of dependent variables and b is an m-vector of parameters. To solve this type of optimization problem, two strategies can be followed, the method of extreme points and the method of interior points, depending on which part of the feasible region is explored to find the optimal value. The first method is called the Simplex method (Dantzig, 1963), while the second procedure is called the interior point method (Bertsimas & Tsitsiklis, 1997). Although each method can be more efficient for a particular problem, the most widely used commercial solvers such as CPLEX and Gurobi include both methods.

Nonlinear programing (NLP)

If the objective function or some of the constraints include nonlinear functions, the optimization problem is called nonlinear programming (Kubn, 1976). In this case, the general mathematical formulation would be the one shown by Eq. (1.19).

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & h(x) = 0 \\ & g(x) \leq 0 \\ & x \in X \subseteq \Re^n \end{aligned} \tag{1.19}$$

Where f(x) is the objective function of the problem, h(x) is the set of equality constraints and g(x) is the set of inequality constraints. To solve this type of optimization problem, 3 strategies can be followed, successive quadratic programming (SQP), reduced gradient algorithms, and interior point methods.

- SQP algorithms solve the quadratic program of the original function and linearize the constraints, determining at each interaction the Newton step and Lagrange multipliers to decide the direction of the optimal value search and ensure convergence.

- Gradient reduction methods use an approximation of the original constraints and reduce the number of variables to reduce the dimension of an original problem, to which Newton's method is applied to find the optimum. In each interaction, the search direction is corrected based on the calculated gradient, minimizing the objective function.

- Finally, interior point methods use relaxed variables to replace the inequations by 'y' equations and the log-barrier function to handle the non-negativity of the 'x' variables. Once relaxed, the first-order Karush-Kuhn-Tucker (KKT) conditions and Newton's method are used to solve the optimization problem.

SNOPT (Gill et al., 1997) and fmincon (Mathworks, 2007) use SQP (Biegler, 2010), MINOS (Murtagh & Saunders, 1983) and CONOPT (Drud, 1996) use gradient reduction methods; and IPOPT (Wächter & Biegler, 2006) and KNITRO (Byrd et al., 2006) use interior point methods. Depending on the nature of the nonlinearities in the model, one or the other method will be more effective. Most mathematical models that integrate process, product, or control design are of this type. Integrated product and process design applied to formulated products can be integrated into a mathematical NLP optimization model. Linearization techniques (piecewise linear approximation) and techniques aimed at eliminating bilinear products, such as Mc-cornick envelopes, can be used before applying a commercial solver. This not only reduces the computational time needed to find an optimum but can also allow for finding a solution to a problem that could not be solved directly.

Mixed-integer linear programming (MILP)

This type of optimization problem is similar to the linear problem but considers that one or more variables are integers. The mathematical formulation is presented by Eq.(1.20).

$$\begin{aligned} \min \quad & Z = a^T x + b^T y \\ \text{s.t.} \quad & Ax + By \leq d \\ & x \geq 0 \quad y \in \{0,1\}^m \end{aligned} \tag{1.20}$$

Where 'y' are discrete variables and 'x' are continuous variables. In this case, 4 methods have been followed to find an optimal value, cutting planes, Benders decomposition, Lagrangian Decomposition, Branch and Bound search, and Branch and Cut methods (Grossmann, 2021).

Cutting planes uses a linear relaxation of the original problem along with a series of cutting planes that bound the solution in each iteration, excluding the non-feasible solutions of the original MILP through the constraints (Floudas, 1995). One particular class of cutting planes is the covering inequality (CI). CI was introduced independently by Balas (Balas, 1975), Hammer et al. (Hammer et al., 1975) and Wolsey (Wolsey, 1975) and were defined for 0-1 Knospsack type problems, although they were later extended to any linear 0-1 problem. This methodology consists mainly in introducing linear inequalities to reduce the feasible region to which to apply the cutting planes.

In each iteration, the Bender decomposition will bind the feasible region of the problem creating new upper and lower values of the optimal solution. The upper value is calculated by solving the problem as if it were an LP by fixing the integer variables. The lower value is computed by generating LP problems derived from the original problem, through duality theory.

Lagrangian decomposition (Monique & Siwhan, 1987), also known as variable splitting, is a specific form of Lagrangian relaxation. Lagrangian relaxation consists of eliminating (relaxing) one or more constraints and penalizing violations of these constraints in the objective function by means of coefficients called Lagrangian multipliers. This generates a series of subproblems where the remaining uncomplicated constraints are duplicated in each of these subproblems. The solution of these subproblems generates different upper bounds.

Branch and Bound methods create a tree with each discrete decision marked by the values of the binary variables considered in the problem (see Figure 1.6). To solve the problem, the original model is relaxed to an LP model. If the solution of the binary variables is an integer, the optimal value has been found, otherwise, two branches of the tree are generated, one for each value of the binary variable set. The process is repeated until the optimal value is found. Heuristic rules and gradient analysis are used to avoid generating all possible branches and simplify the tree.

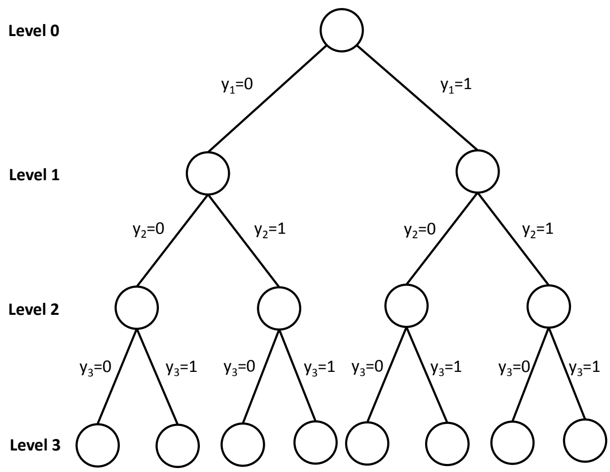

Figure 1.6: Decision tree from a branch and bound algorithm

Branch and Cut methods combine the Branch and Bound method with the cutting plane method to facilitate the convergence of the model. Cutting planes are added in relaxed problems to adjust the solution towards the integer value of the variable and reduce the convergence time.

These solving methods for MILP problems are often integrated into commercial algorithms such as CPLEX (ILOG, 2009) and Gurobi (Gurobi Optimization, 2021).

Mixed-integer nonlinear programming (MINLP)

These are the most complex models to solve from the optimization point of view since they combine the problems of including discrete variables together with nonlinear functions or restrictions. Their general mathematical expression is shown by Eq.(1.21):

$$\begin{aligned}
\min \quad & f(x,y) \\
\text{s.t.} \quad & h(x,y) = 0 \\
& g(x,y) \leq 0 \\
& x \in X \subseteq \Re^n \\
& y \in \{0,1\}^m
\end{aligned} \tag{1.21}$$

To solve this type of optimization problem, different strategies have been proposed, among which the generalized Bender decomposition (GBD), the outer approximation (OA), the extended cutting planes (ECP), and the generalized cross decomposition stand out.

All the methods presented generate sequences of lower and upper bounds, which converge to the solution. The difference between one and the other lies in how these limits are calculated. The upper bound is calculated by setting the 'y' variables in the GBD (Geoffrion, 1972), ECP (Westerlund & Pettersson, 1995), and OA (Duran & Grossmann, 1986).

On the other hand, the lower bound is fixed in different ways depending on the method, although all of them follow strategies to linearize the original problem with the fixed binaries and seek to obtain information about which binary variables should be fixed in the next iteration to converge to the optimal solution. For instance, the OA, the lower bound is obtained through a linearization of the nonlinear objetive and constraints function around the primal solution while ECP replaces the NLPs of the primal problem by a simple function evaluation.

The Branch and Bound and Branch and Cut methods can also be applied to MINLP as long as the number of binary variables is not too large, solving at each node an NLP through the strategies described above (see the NLP section).

The development of superstructures that simultaneously consider several physical and/or chemical transformation processes involves MINLP-type models. In some cases, binary variables can be replaced by continuous variables. This is usually the case for those models that only consider operating costs and not investment costs. This is because the fixed costs of a process are included or excluded from the final cost of the plant depending on the value of the binary variable (0 if not included and 1 if included). It is possible to scale investment costs with continuous variables such as production or treatment capacity (q) using potential expressions (q_C) that consider economies of scale in costs, where c is usually 0.6 in the chemical industry. However, these types of expressions make the mathematical solution of the optimization problem more difficult by introducing non-linear and non-convex expressions.

Integrated product, process, and supply chain systems also often involve MINLP models in which substitution of binary variables is not possible. In this case, efforts can be focused on decomposing the problem or linearizing the nonlinear functions or bilinear products, (Lagrangean or Benders decomposition (Conforti et al., 2014)). Nonlinear equations are more complicated to avoid because the mass and energy balances, as well as, thermodynamic equilibrium have bilinear products, and quadratic or logarithmic equations.

1.7 STRUCTURE OF THE THESIS

This thesis is presented as a compendium of scientific articles and, therefore, each of these articles constitutes a chapter of this thesis. Format changes are only considered with respect to published (or in process of publication) scientific articles in order to unify and standardize the thesis. The supplementary material of each article will be included in the thesis through appendices. The thesis will be divided into two parts:

Part 1: In this part, the integrated design of products, processes, and supply chains will be analyzed for the particular case of formulated products. While in the first chapters (chapters 1 and 2) integrated design will be applied to the manufacture of detergents, in chapters 3 and 4 it will be applied to the integration of the livestock and agricultural industry through optimal design of feed and fertilizers.

Chapter 3: As an intermediate step to the integration of the supply chain to detergent design, the effect of supplier selection on the economic and environmental impact of powder detergent production will be evaluated.

Chapter 4: The integrated product, process, and supply chain design for detergent powder manufacturing at the continental level and the development of methodologies to find an optimal solution in a reasonable computational time will be addressed.

Chapter 5: The integration of a livestock system and a crop production system will be analyzed, through the optimal design of the animal feed (which will be produced in the same facility) and the treatment of animal waste (which will be used to supply part of the nutrients necessary for crop growth) favoring the circular economy between both industries.

Chapter 6: The location and sizing of integrated livestock-farming systems will be analyzed, and how these new dimensions of the problem affect the design of the facility, integrated product design (feed), process design (animal digestion, crop management and waste treatment), and supply chain (location and sizing).

Part 2: This second part will address the design of the product,the process, and the problem of locating facilities for waste valorization.

Chapter 7: The different industrial alternatives for the valorization of one of the most important residues in coffee production, the spent coffee ground, will be analyzed according to its composition and the production capacity of the plant, as well as the available budget.

Chapter 8: The different alternatives at the industrial level will be analyzed, from an economic, environmental, and social points of view, for the valorization of the 'grape pomace' generated in the production of wine. The best process will be established according to the composition of the grape pomace, the production capacity, and the capital to be invested.

Chapter 9: Through a multi-scale analysis and analyzing 4 different types of waste and 2 treatment processes, the potential for natural gas self-sufficiency that a country can achieve through the valorization of its waste will be analyzed. Based on the composition and performance of the process, the size, type, and location of the treatment plants will be established according to the budget allocated to waste treatment.

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2

OBJECTIVES

The objective of this thesis is to address the integrated process, product, and supply chain design for added-value products. This integration presents a series of problems that is addressed through the development of mathematical models and methodologies. Each of them is evaluated using practical cases representative. Therefore, the main objective is split into a series of specific objectives, which are presented below.

- integrating in a single mathematical model the design of the detergent powder, its production process, and its supply chain, in order to simultaneously determine the optimal composition, the best operating conditions of the production process, as well as the best place to locate production plants, raw material suppliers and customers, from both economic and environmental points of view.
- Designing methodologies (such as linearization processes, initialization of variables, problem decomposition, etc.) that allow addressing and solving very large mixed integer non linear mathematical problems in a reasonable computation time.
- Developing strategies to implement a circular economy that integrates the meat and the crop production systems, through sustainable animal feed design and the treatment of the animal waste.
- Evaluating integrated and decouple systems from economic and environmental perspectives at process, product, and supply chain levels.
- Analyzing the application of integrated product and process design to the valorization of agri-food waste, considering a series of treatment processes and the production of added-value products (superstructure design) and selecting the optimum from an economic, environmental and social points of view.
- Using the integrated design of products and processes to increase the energy security of a country through the production of biomethane from the treatment of agricultural and human waste.

- Evaluating representative case studies to analyze the importance of considering waste composition in the design, optimization, and selection of treatment processes.
- Generalizing the methodologies so that they can be easily applied to other case studies.

Part I

ADDED-VALUE PRODUCTS FROM FORMULATED PRODUCTS

3

ON THE EFFECT OF THE SELECTION OF SUPPLIERS ON THE DESIGN OF FORMULATED PRODUCTS

ABSTRACT

An extended pooling problem is developed for the design of detergents, that include process and product design together with suppliers' selection. It is a multi-period and multi-objective optimization problem since it considers the economic benefit and environmental impact as well as the contract length. This problem can be considered as a previous step to the integrated product, process and supply chain design. This type of problems is non-linear and non-convex. Two formulations are developed to tackle this problem. An MINLP and a reformulated NLP using a decision vector avoiding the use of binary variables. The NLP shows better computational performance in spite of the larger problem size. Furthermore, it is demonstrated that when considering different ingredients, formulations, pricing policies and suppliers, their selection can be adjusted until a reduction of almost 40% of CO_2 emissions is achieved without the benefit decreasing more than 1.5%.

Keywords: Integrated process, Product design, Supplier selection, Multi-objective optimization

RESUMEN

Se desarrolla un problema de agrupamiento extendido para el diseño de detergentes, que incluye el diseño de procesos y productos junto con la selección de proveedores. Es un problema de optimización multiperíodo y multiobjetivo, ya que considera el beneficio económico y el impacto ambiental, así como la duración del contrato. Este problema puede considerarse como un paso previo al diseño integrado de productos, procesos y cadenas de suministro. Este tipo de problemas es no lineal y no convexo. Se desarrollan dos formulaciones para abordar este problema. Un MINLP y un NLP reformulado utilizando un vector de decisión que evita el uso de variables binarias. El NLP muestra un mejor rendimiento computacional a pesar del tamaño del problema más grande. Además, se demuestra que al considerar diferentes ingredientes, formulaciones, políticas de precios y proveedores, su selección se puede ajustar hasta lograr una reducción de casi el 40% de las emisiones de CO_2, sin que el beneficio disminuya más del 1.5%.

Palabras clave: Proceso integrado, Diseño de productos, Selección de proveedores, Optimización multiobjetivo.

3.1 introduction

The market for consumer products is more competitive than ever as a result of globalization. For a product to be competitive, it has to meet specific consumer needs and likes. Therefore, the first stage to design any consumer product consists of identifying those needs and wishes and convert them into physico-chemical properties of the product (Moggridge & Cussler, 2000; Cussler et al., 2010; Uhlemann & Reiss, 2010; Bagajewicz et al., 2011; Teixeira et al., 2012; Tijskens & Schouten, 2014). To optimize this step, the new products can be designed using computer-aided tools and virtual experiments. The systematic approach for the design of products has been applied to the manufacture of polymers (Vaidyanathan et al., 1998), refrigerants (Churi & Achenie, 1997), repellents (Conte & Gani, 2011), and surfactants (Mattei et al., 2014) including social and environmental concerns lately to attract a more conscious consumer (Yue et al., 2013; Garcia & You, 2015; Mota et al., 2015). Subsequently, a process is to be put together that is capable of producing the expected product or a family of products to satisfy the consumer demand. However, the appropriate method to design a new product is to simultaneously consider the product and the production process, allowing a global analysis of the whole process from the conceptual idea of the product to its delivery to the customer (Gani, 2004; Martín & Martínez, 2013; Ng & Gani, 2018) analyzing the trade-offs between the quality of the product and the need of the manufacturing process (Taifouris et al., 2020). In this way, the technical, economic, environmental and safety analysis (Scruggs, 2013; Lacasa et al., 2016) are taken into account not only for the design of the product but also for its production. This allows adjusting the production costs of the products and increasing the competitiveness of the company (Zaman et al., 2018).

A particular case of products is the so-called formulated products. This type of products consists of a mixture of ingredients that altogether are capable of providing the features the consumer expects (Zhang et al., 2017). The integrated approach for the design of products is particularly important in the design of formulated products since the product composition can be modified easily affecting its production process. Therefore, the simultaneous design of the process and the product allows reducing the feasible set of formulas (Bernardo & Saraiva, 2005; Martín & Martínez, 2013, 2018) eliminating those that are not economically and environmentally viable. As a result, the physical resources can focus on the most promising products. On the one hand, the manufacture of formulated products can be approached using an extended pooling problem. In the pooling problem, a series of ingredients are mixed to obtain a product with properties that meet the customers' expectations (Audet et al., 2004). When a pooling problem is mathematically formulated, the presence of bilinear terms in the product quality, composition and the mass balances as well as the functions that model cost estimations (Audet et al., 2004), and process constraints (Martín & Martínez, 2013) makes it highly non-linear. This fact represents a challenge when addressing the integration of the pooling problem within the supply chain. Supply chain studies are typically mixed integer linear programming (MILP) problems where the process and product design have been fixed (Yue et al., 2013). Supply chains including nonlinear terms are most of the times linearized and/or decomposed to make them computationally tractable (Terrazas-Moreno et al., 2012) but this is an approximation of the original problem that for formulated products presents drawbacks. In addition, due to the mathematical complexity, pooling problems are not integrated with the supply chain, which means that it is not possible to ensure that the design of the process and the product are optimal since both are affected by the supply chain. A stage prior to the integration of the complete supply chain would be to integrate the selection of suppliers. Extensive research work on supplier selection has been carried out (Sawik, 2013; Gou et al., 2014; Qian, 2014) studying how the supply chain is affected by these decisions. Nevertheless, the effect of these decisions on product and process design has not been considered yet. In addition, for the economic evaluation of the production process it is necessary to differentiate between two types of ingredients. Those whose price varies with the market and therefore is subjected to the uncertainty of the market and those that can be fixed by multi-period contracts of several years. To account for the variability, studies that introduce uncertainty in the optimization model have been presented (Kim et al., 2011; Martín & Martínez, 2015) while in the case of ingredients with a deterministic price, different pricing policies have been evaluated to estimate the cost of the ingredient depending on the amount of ingredient (Martín & Martínez, 2018). While both considerations have been analyzed separately, either ingredients prices with associated variability (Martín & Martínez, 2015) or ingredients whose price is fixed by multi-period contracts (Martín & Martínez, 2018), the most realistic case would be an intermediate case in which some of the prices of the ingredients are fixed by contracts and others have an associated market variability.

In this work, we integrate the selection of suppliers into the integrated process and product design problem for a specific case of formulated products, powder detergents. Therefore, it is a step towards the integration of product design, process and supply chain in formulated consumer products. Two objectives will be taken into account, the economic benefit and the environmental impact. This type of problem is complex and requires an analysis to address it in order to consider the impact of the environmental impact on the benefit, the optimal formulation of the product, the selection of suppliers and the selection of pricing policies. The optimization model developed, which is multi-objective and multi-period, seeks to analyze the trade-off between the economic benefit as the environmental impact limit and the effect on a wide variety of decision variables such as the amount and type of purchased raw material, suppliers and price policies. The rest of the paper is organized as follows. In Section 3.2, the mathematical optimization model is developed including the formulation of the process, the ingredients considered and the price estimation method, whether fixed by contracts or subject to market variability, the estimation of the environmental impact index and the main objective function.The two formulations considered are presented. In Section 3.3, the model is applied for a case study in Europe. In Section 3.4, the results are shown and in Section 3.5, the conclusions and future work are discussed.

3.2 MATHEMATICAL MODEL

3.2.1 *Problem description*

We address the sustainable production of three types of powder detergents with different performances and prices, from economic and environmental points of view. In addition, to integrate the process and product design with the supply of the ingredients, we seek to analyze the effect of the selection of different suppliers on both objectives. Several suppliers are considered for each type of ingredient, with different distances between the suppliers and the factory and different prices related to those distances. The environmental impact associated with the transport is also considered. The detergent performance is introduced as a constraint with minimum and maximum values for each type of detergent. In an attempt to get closer to reality, 7 groups of ingredients are considered. These groups include the most used ingredients in industry (Ecolabel, 2009). 17 ingredients with different environmental impacts and prices are evaluated, see Table 3.1.

Table 3.1: Ingredients considered

Group	Ingredient	Abbreviation
Surfactant	Linear alkyl aryl sulfonates	LAS
	Alcohol ethoxylates and Alkyl amides	AE
	Esterified mono-alkyl	MTEA
Builder	Polyphosphates	STPP
	Zeolite	ZE
Bleach	Sodium perborate tetrahydrate	S. PERBO
	Sodium percarbonate.	S. PERCA
Fillers	Sodium sulfate	S.SU
	Xylene sulphonate	X.SU
Antifoaming agents	-	ANTI
Enzymes	Protease	PRO
	Lipase	LIP
	Cellulose	CELL
Polymers (Antiredeposition agents)	Carboxymethyl cellulose	CMC
	Sodium polyacrylate	S. POLY
	Polyethylene glycol	POLYGLY

In addition, the price of some ingredients can be arranged through multi-period contracts (3 years) and others have an associated market variability. For those whose price is fixed throughout the year, the best pricing policy is to be selected based on the amount used. The final product is obtained by mixing the ingredients as long as processing and performance constraints are met including particle size and cake strength. Both types of constraints are modeled as a function of the concentration of the ingredients as in previous works but updated to account for the use of different ingredients within the same group.

Over the years, tighter environmental regulations have been passed. To evaluate the effect of the ever-decreasing emission limits, the environmental impact of the production of the final products is computed. By using the ϵ-constraint method, the trade-off between the profit and the environmental impact due to the ingredients and their transportation is evaluated. Therefore, a mathematical model is developed that takes into account the mass balances of the detergent production process, the limitations associated with this process, the calculation of the performance of the final product, the environmental impact of the ingredients and their transport, and ingredient pricing policies, purchased through contracts and the price of ingredients with associated uncertainty. For the sake of the length of the work, we refer the reader to previous works for details on the modelling of the process constraints (Martín & Martínez, 2013, 2018).

3.2.2 *Model development*

In this section, two different formulations of the problem are described. The original one is an extension of the work of Martín and Martínez, 2015, 2018 based on a mixed integer non-linear programming (MINLP) formulation. However, the complexity of the problem and the expected extension to address the entire supply chain suggest a different solution approach. Therefore, an alternative formulation is also developed.

3.2.2.1 *Production process*

The mathematical formulation for the design of detergents used in this work is based on the model presented by Martín and Martínez, 2013. The ingredients follow five stages: the mixture of the ingredients where a series of physico-chemical reactions is favored, the atomization of the slurry to avoid possible jams, a drying process in a spray drier, a cooling process and a finishing stage where a series of additives is added to adjust the properties. We refer the reader to previous work of Martín and Martínez, 2013 for the complete process. In this work, the formulation is updated to account for various ingredients within the same group and several suppliers per ingredient.

3.2.2.2 *Mass balances and process constraints.*

In order to follow the mass balances and the rest of the sections presented below, it is necessary to explain the difference between the 'i' index, which represents the types of raw materials that are fed to the plant and previously purchased from the suppliers; and the 'k' index that represents the pure ingredients. In this work, it has been considered that the raw materials only contain a single ingredient, so that the flow i = 1 only contains the component k = 1 (same for the rest). However, formulating the model in this way allows the raw material to be composed of different ingredients (in previous work, some of these flows of raw materials had several ingredients because they were residues of other processes).

The purchased amount of the raw material is related to the inflows to the factory, given by Eq.(3.1).

$$\sum_{sup} ccp_{ye,i,sup} = \sum_{l} x_{ye,i,l} + \sum_{j} z_{ye,i,j} \tag{3.1}$$

Where $\text{ccp}_{ye,i,sup}$ is the amount purchased in the year "ye" of the raw material "i" from the supplier "sup". It is not necessary to use binary variables for the selection of suppliers because the variable $ccp_{ye,i,sup}$ will select to buy the optimal amount of raw material 'i' from the best supplier, considering the availability, the distance, the prices and the rest of variables that influence it. In this way, if the necessary amount of raw material 'i' can be purchased from a single supplier, only one will be selected (the optimal one), be cause centralizing purchases will reduce the prices of the raw material by economies of scale (see Eqs.(3.30)-(3.33)). But if a single supplier cannot supply the needs of a raw material, the model will proceed to buy first to the optimum and then to the second best.

It is necessary to differentiate between the limits imposed by each of the suppliers according to their own capacity ($Lsup_{i,sup}$ and $Linf_{i,sup}$) and the inherent limits to the process (Au_i and Al_i):

Nevertheless, by default we consider that there is no maximum or minimum production limit. However, in this work these limits will be fixed by the maximum and minimum amount of raw material available. The differentiation between the limits is maintained for the model to be generic. In this way, if it is necessary to set a production capacity limit, the model will not need important changes. Therefore, we include Eqs.(3.2) and (3.3) in the model.

$$\sum_{sup} Lsup_{i,sup} = Au_i \tag{3.2}$$

$$\sum_{sup} Linf_{i,sup} = Al_i \tag{3.3}$$

The sum of the flows of raw materials that go to the intermediate tanks and those that go to the final product tank must be between the upper and lower limit of the process Eq.(3.4).

$$A_i^L \leq \sum_l x_{ye,i,l} + \sum_j z_{ye,i,j} \leq A_i^U \tag{3.4}$$

As it can be seen, all these limits are not per unit of time because the same limits are assumed every year. The total amount sent to the intermediate tanks must be less than or equal to the maximum capacity of the intermediate tank (Eq.(3.5)).

$$\sum_l x_{ye,i,l} \leq S_l \tag{3.5}$$

The amount of detergent produced must be between the maximum and minimum limit of the detergent demand (Eq.(3.6)).

$$D^L_{ye,j} \leq \sum_l y_{ye,l,j} + \sum_i z_{ye,i,j} \leq D^U_{ye,j} \tag{3.6}$$

The demand depends on the period since the demand for the first year may be different from the demand in second year depending on the result of the market study in the region of study. Eq.(3.7) shows the mass balances to intermediate tanks.

$$\sum_i x_{ye,i,l} = \sum_j y_{ye,l,j} \tag{3.7}$$

The mass balances to the different ingredients between the input streams and the intermediate tanks are shown by Eq.(3.8).

$$\sum_i CC_{i,k} \cdot x_{ye,i,l} = \sum_j p_{ye,l,k} \cdot y_{ye,l,j} \tag{3.8}$$

Where $CC_{i,k}$ is the initial concentration of component 'k' of the raw material streams 'i' and $p_{ye,l,k}$ is the concentration of component 'k' in tank 'l' in year 'ye'. It is considered that the initial concentration of the raw material streams will be the same every year. It does not depend on the time period or the chosen supplier.

To establish the limits of the composition of each ingredient 'k' in the final product, a new dimension is defined since the limits, both lower and upper, will be set taking into account the group to which it belongs and not the particular ingredient. In this way, there are common limits to different chemical substances depending on whether they are surfactants, builders, bleaches or the rest of groups. Thus, within each group, the mathematical model can choose a different amount of each ingredient of the same group (in order to meet the expected properties) with respect to the limits of the group. For example, in the case of the group 'surfactants', there will be an upper and a lower limit for the sum of the three different surfactants, but not for LAS, AE or MTDI individually. Thus, the composition can be properly adjusted. Therefore, a new dimension is defined, corresponding to the group 'g', and upper and lower limits are established for each group. The equivalences between the minimum and maximum compositions of each group and the sum of the different ingredients are shown by Eqs.(3.9)-(3.16).

$$P^L_{j,1} \leq \left(PQ_{j,1} + PQ_{j,2} + PQ_{j,3}\right) \quad \leq \; P^G_{j,1} \tag{3.9}$$

$$P^L_{j,2} \leq \left(PQ_{j,4} + PQ_{j,5}\right) \;\; \leq \; P^G_{j,2} \tag{3.10}$$

$$P^L_{j,3} \leq \left(PQ_{j,6} + PQ_{j,7}\right) \leq P^G_{j,3} \tag{3.11}$$

$$P^L_{j,4} \leq \left(PQ_{j,8} + PQ_{j,9}\right) \; \leq P^G_{j,4} \tag{3.12}$$

$$P^L_{j,5} \leq PQ_{j,10} \;\; \leq \; P^G_{j,5} \tag{3.13}$$

$$P^L_{j,6} \leq \left(PQ_{j,11} + PQ_{j,12} + PQ_{j,13}\right) \;\; \leq \;\; P^G_{j,6} \tag{3.14}$$

$$P^L_{j,7} \leq \left(PQ_{j,14} + PQ_{j,15} + PQ_{j,16}\right) \leq \; P^G_{j,7} \tag{3.15}$$

$$P^L_{j,8} \leq \left(PQ_{j,17}\right) \leq \;\; P^G_{j,8} \tag{3.16}$$

These limits are considered to be constant over the periods of time, just like the optimal formulation of the final product. The global balance of ingredients is given by Eq.(3.17).

$$PQ_{j,k} \;\cdot \left(\sum_l y_{ye,l,j} + \sum_i z_{ye,i,j}\right) = \sum_i CC_{i,k} \cdot z_{ye,i,j} + \sum_l p_{ye,l,k} \cdot y_{ye,l,j} \qquad \forall ye, j, k \tag{3.17}$$

The limits of each stream are given by Eqs.(3.18)-(3.20).

$$0 \leq x_{ye,i,l,t} \leq min \left\{ A^U_i, S_l, \sum_j D^U_{ye,j} \right\} \tag{3.18}$$

$$0 \leq y_{ye,l,j,t} \leq min \left\{ S_l, D^U_{ye,j}, \sum_i A^U_i \right\} \tag{3.19}$$

$$0 \leq z_{ye,i,j,t} \leq min \left\{ D^U_{ye,j}, A^U_i \right\} \tag{3.20}$$

In addition, it is necessary to include the surrogates that predict the product performance, the environmental impact and the process constraints.

3.2.2.3 *Calculation of the product performance.*

To determine the effect of the concentration of ingredients in the final product on the performance, a design of experiments (DOE) was formulated using open literature data to evaluate which ingredients were the ones that were most likely to affect the cleanliness of the clothes. Using those data, a correlation was obtained and used in the mathematical model. For more details on how the correlations were developed, see the work of Martín and Martínez, 2013. Assuming that the different types of surfactants, enzymes, builders, polymers and bleaches have the same effect on the performance, the original formulation of the work of Martín and Martínez, 2013 was modified and Eq.(3.21) is obtained.

$$\begin{aligned} Performance_j = (107 \cdot (PQ_{j,surf1} + PQ_{j,surf2} + PQ_{j,surf3}) + \\ 1872 \cdot \left(PQ_{j,enz1} + PQ_{j,enz2} + PQ_{j,enz3}\right) + \\ 53.9 \cdot \left(PQ_{j,bu1} + PQ_{j,bu2}\right) + \\ 134 \cdot \left(PQ_{j,pol1} + PQ_{j,pol2} + PQ_{j,pol3}\right) + + \\ 119 \cdot \left(PQ_{j,bl1} + PQ_{j,bl2}\right) \end{aligned} \tag{3.21}$$

The quality of the detergent is directly related to the value of the performance. To identify three detergents, three different performances are established:

- Detergent A (High quality and high price) $\geq$ 0.95
- Detergent B (Average quality and average price) $\geq$ 0.80
- Detergent C (Suficient quality and lower price) $\geq$ 0.70

Note that a more detailed correlation can be developed to evaluate the effect of each ingredient but, due to confidentiality issues and the difficulty in making up a reasonable correlation, we used this correlation for the model formulation.

3.2.2.4 *Process constraints*

The detergent production process has a series of constraints related to the processing of the mixture and the final product. To estimate a correlation that relates the concentration of the ingredients in the final product to the particle size and cake strength, the same procedure was followed as in the case of the performance. On the one hand, the particle size can neither be larger than 500 μm nor smaller than 400 μm (Bayly et al., 2006). This size determines the correct dissolution of the detergent in water within the washing machine. To estimate the particle size (μm) as a function of the composition, Eq.(3.22) is used.

$$Particle_j = 224.5 + 1509.78 \cdot PQ_{j,water} + 1000 \cdot \left(PQ_{j,filler1} + PQ_{j,filler2}\right) - 31 \cdot PQ_{j,water} \cdot \left(PQ_{j,filler1} + PQ_{j,filler2}\right) \tag{3.22}$$

On the other hand, for the detergent to be functional, the cake strength should be below 1 kg (Ebihara & Watano, 2003). To determine the cake strength(kg), Eq.(3.23) is used.

$$Cakest_j = 2.98 \cdot PQ_{j,water} + 2.69 \cdot \left(PQ_{j,poly1} + PQ_{j,poly2} + PQ_{j,poly3}\right) + 0.08 \cdot PQ_{j,water} \cdot \left(PQ_{j,poly1} + PQ_{j,poly2} + PQ_{j,poly3}\right) \tag{3.23}$$

3.2.2.5 *Implementation of environmental impact*

The location of the suppliers of raw materials does not only affect the production cost, but also the environmental impact associated with the production of the final product. The environmental impact of a chemical can be evaluated with different indexes depending on the focus of the analysis. On the one hand, there are exhaustive studies where all the possible impacts of a chemical are analyzed throughout its life cycle, that is, from the order of the raw materials, their transportation, the production process, the packaging, its distribution and use. These studies are called Life Cycle Assessment (Saouter & Hoof, 2002). On the other hand, the Ecolabel (Ecolabel, 2009) evaluates the pollution that a chemical can cause to the aquatic environment. It is evaluated as the critical dilution volume, which represents the amount of water necessary for the impact of that substance to be negligible in the medium to which it is released. Therefore, this index evaluates the impact that the detergent may generate as a result of its manufacture and use, and when it is released to the sewage. In other to analyze the environmental impact in the atmosphere in the form of emissions of greenhouse gases, the carbon footprint (organization, 2017) is typically used (Gong & You, 2014; Peng et al., 2019; Ai et al., 2020) . Each ingredient used to produce a detergent has a carbon footprint associated with its own production process and the sum of all these results in the carbon footprint of the production of the detergent. The emissions generated by the transport of the raw material from suppliers to the factory are the second contribution to the footprint. In this work, only the carbon footprint will be used.

To evaluate the carbon footprint, the distance between suppliers and the factory must be considered.The emissions are estimated to be approximately 0.5 kgCO_2/km (Commission, 2018). Therefore, the emissions due to goods shipping will be calculated as indicated in Eq.(3.24).

$$Emission_{sup} = distance_{sup} \cdot 0.5kgCO_2/km \quad \forall sup \tag{3.24}$$

The unit emission associated with transport is calculated as indicated in Eqs.(3.25) and (3.26).

$$EmissionU_{sup} = \frac{Emision_{sup}}{Loading\ capacity} \quad \forall sup \tag{3.25}$$

$$Emision\ T_{ye,sup} = EmisionU_{sup} \cdot \sum_i ccp_{ye,i,sup} \ \ \forall ye, sup \tag{3.26}$$

The loading capacity value is set to 7t, while the carbon footprint associated with the different ingredients can be calculated from the composition of the final product (Eq.(3.27)):

$$\mathrm{HC}i_{ye}\,(\mathrm{kg}CO_2eq) = \sum_{j,k} MassProd_{ye,j} \cdot PQ_{j,k} \cdot HCK_k \quad \forall ye \tag{3.27}$$

Where $\mathrm{MassProd}_{ye,j}$ is defined by Eq.(3.28).

$$MassProd_{ye,j} = \sum_l y_{ye,l,j} + \sum_i z_{ye,i,j} \quad \forall ye, j \tag{3.28}$$

HCK_k is the carbon footprint associated with the ingredients.

This value can be found in the supplementary material. To determine this value, the manufacturing process of each ingredient is evaluated, focusing on the energy consumed to produce them and how that energy is provided, that is, if either natural gas, coal, oil or steam is used. Based on these two parameters, the carbon footprint associated with the manufacturing process is computed. It also evaluates whether CO_2 or other greenhouse gases are released in the process due to the chemical reactions involved. In this way, this index assesses the impact on the atmospheric environment produced by the gases released in the production process.

The total carbon footprint will be computed using Eq.(3.29).

$$\mathrm{HC}_{ye} = \mathrm{HC}i_{ye} + \sum_{sup} Emision\ T_{ye,sup} \quad \forall ye \tag{3.29}$$

3.2.2.6 *Calculation of raw material and transportation cost*

For a more realistic estimation of the price of the raw material, two cases are considered. On the one hand, the price of certain ingredients can be fixed through contracts with the suppliers, using pricing policies with discounts that will depend on the amount purchased. A wide variety of pricing policies associated with raw materials sales contracts have been presented in the literature. Some studies have evaluated the selection of the types of contracts for each situation (Tsay et al., 1999; Park et al., 2006; Bansal et al., 2007; Höhn, 2010; Khalilpour & Karimi, 2011) . Other authors have studied them from the point of view of the supply chain (Park et al., 2006; Calfa & Grossmann, 2015). In this model, four different discount policies are considered for each supplier according to the amount of raw material used. However, there will be ingredients whose price is more variable throughout the year and cannot be fixed in the long term. In this case, it will be necessary to assume that there exists a market variability associated with the price. In addition, the price of the raw material of each supplier will depend on the distance so that those suppliers that are further away have a lower ingredient price than the nearest ones. Ingredient prices also depend on the environmental impact associated with the ingredient contained in the raw material of the supplier. The more polluting the ingredient is, the cheaper it will be.

3.2.2.7 *Assessment of market price variability*

In this study, only exogenous uncertainty is considered, which is the uncertainty imposed by external factors such as the market (supply and demand (Govindan & Fattahi, 2017)) on the sale prices of the product or the prices of the ingredients (Martín & Martínez, 2015). However, in the literature, you can find different authors (Sahinidis, 2004) that implement uncertainty within their models through the use of scenarios. The probability of each uncertain value is computed from the probability distribution function of each one. With that, it is possible to compute the probability of each scenario and the price/demand associated with it. However, the number of possible scenarios to represent the probability distribution is typically extremely large, so scenario reduction techniques are used. Some examples of these techniques have been proposed by Karuppiah et al., 2010 and Liz and Li and Floudas, 2014. These techniques were applied to product design in previous work (Martín & Martínez, 2015). For this work, even using the scenario reduction techniques, as it is necessary to evaluate each of the variables of the model for each of the scenarios, the model becomes computationally unsolvable. The large and complex problem when suppliers are considered lead to the use of an average price for those ingredients that present market variability using the probability. This approach follows from the findings in Martín and Martínez, 2015 where the optimization using the average price and that using the scenarios showed similar results. It will be considered that the prices with market variability are the surfactants, antifoams and polymers. Three levels of prices are used for each ingredient, high, medium or low. The average price is computed using their associated probabilities.

3.2.2.8 *Selection of the pricing policies*

The equations necessary to calculate the discount in each of the price policies considered are given by Eqs.(3.30)-(3.33).

These expressions were obtained from previous works (Martín & Martínez, 2018) and modified to adapt them to the current formulation.

P1 Linear discount: The discount applied to the original price follows a linear profile based on the amount of raw material purchased:

$$costj_{ye,i,sup,1} = c0_{i,sup} - \left(\frac{c0_{i,sup} \cdot discount}{Lsup_{i,sup} - Linf_{i,sup}} \right) \cdot (ccp_{ye,i,sup} - Linf_{i,sup}) \forall ye, i, sup \tag{3.30}$$

co$_{i,sup}$ is the initial price of the raw material 'i' from the supplier 'sup', L$_{sup,i}$, and Linf$_{i,sup}$ are the maximum and minimum amount of raw material 'i' that can be purchased from the supplier 'sup'. 'discount ' is a parameter of the policy that must be negotiated with the company and that will set the maximum discount. Note that discount policies only apply to raw materials that can be set by contracts. The costj$_{ye,I,sup,po}$ value for the ingredients subject to variability will be equal to 0.

P2 Logarithmic discount: The discount is the maximum once the amount purchased reaches a certain level, but the decrease is also fast depending on the maximum amount available, Lsup$_{i,sup}$:

$$costj_{ye,i,sup,2} = c0_{po,i,sup} \cdot \left(\frac{1}{1 + disct} \right) + c0_{po,i,sup} \cdot \left(\frac{\left(\exp\left(- \left(\left(\frac{1}{Lsup_{i,sup}} \right) + \left(\frac{10}{Lsup_{i,sup}} \right) \cdot ccp_{ye,i,sup} \right) \right) \right)}{\left(disct + \exp\left(- \left(\left(\frac{1}{Lsup_{i,sup}} \right) + \left(\frac{10}{Lsup_{i,sup}} \right) \cdot ccp_{ye,i,sup} \right) \right) \right)} \right) \tag{3.31}$$

'disct' is a parameter that sets the applied discount.

P3 Constant elasticity: The applied discount is exponential depending on the amount used of the raw material. 'powd' is a model parameter that can be different for each raw material and for each supplier.

$$costj_{ye,i,sup,3} = c0_{po,i,sup} \cdot \left(ccp_{ye,i,sup}\right)^{\left(-powd_{i,sup}\right)} \forall ye, i, sup \quad (3.32)$$

P4 fixed discount: In this case, the discount is independent of the amount of the raw material 'i' used. This type of discount is very appropriate when the amount you are going to buy a raw material is small.

$$costj_{ye,i,sup,4} = c0_{po,i,sup} \cdot (1 - fixdisc) \forall ye, i, sup \quad (3.33)$$

'fixdisc' is the discount parameter of this policy.

The selection of a particular policy depends on the amount purchased and the maximum and minimum amount available for each raw material. In order to reduce the unit cost, the policy that provides the largest discount on the original price will be selected. To select a single reduction policy, it is necessary to introduce Eq.(3.34) and change $co_{i,sup}$ for $c_{po,i,sup}$ in Eqs.(3.30)-(3.33).

$$c_{po,i,sup} - c0_{i,sup} \cdot bi_{po,i} = 0 \quad (3.34)$$

Eq.(3.34) assigns c $_{po,i,sup}$ the value of co $_{i,sup}$ if the policy is selected and the value of 0 if that policy is not taken into account in the final price of the raw material. In addition, only one pricing policy per raw material and per supplier will be selected (Eq.(3.35)).

$$\sum_{I} bi_{po,i} = 1 \quad (3.35)$$

Since at most one must be different from 0 (Eq.(3.35)), the one that assigns the lowest final cost for raw material 'i' as a function of the amount purchased will be selected. If the variability in the price of some of the ingredients is such that it can no longer be fixed by contract, in the formulation this ingredient is assigned to the group of those who have uncertainty without requiring a significant change in the model formulation.

The unit cost will be given by Eq.(3.36).

$$Cost_{ye,i,sup} = \sum_{po} Costj_{ye,i,sup,po} \quad (3.36)$$

The problem is multiperiod. Not only one production year is considered, but several years with different demands from the customers. This means that the price discount will be calculated each year, but the contracts will be made for several years. Therefore, if a particular policy is chosen for the first year, the next one will have to use the same policy. As the binary variable does not depend on the year, once a policy is selected, it will be maintained every year, although the evaluation of the cost of the prices is per year.

3.2.2.9 *Calculation of the unit price of the raw material ingredients.*

The total raw material cost is computed adding the cost of the ones fixed by contracts and those subjected to the market as given by Eq.(3.37).

$$CostP_{ye,i,sup} = cost_{ye,i,sup} + Costf_i \tag{3.37}$$

In this case, the Costf_i represents the average price of the ingredients with uncertainty, being 0 for the ingredients whose price is set by contract. Thus, by adding $\text{Cost}_{ye,i,sup}$ and Costf_i , the resulting price vector, $\text{CostP}_{ye,i,sup}$, contains the price of all ingredients.

3.2.2.10 *Transportation cost*

Transportation is expected to have a considerable impact on annual production costs. The transportation cost for each supplier is calculated by Eq.(3.38).

$$Ctrans_{sup} = distance_{sup} \cdot priceT \tag{3.38}$$

priceT is determined considering a consumption of 25L/100km and a cost of diesel of €1/L, to become 0.25 €/km. The distance will depend on the location of the supplier. The unit cost of transport will be given by Eq.(3.39).

$$CTransU_{sup} = \frac{Ctrans_{sup}}{Loading\ capacity} \forall sup \tag{3.39}$$

And the total transport cost per supplier will be defined by Eq.(3.40).

$$CTT_{sup} = CtransU_{sup} \cdot \sum_{i,ye} ccp_{ye,i,sup} \quad \forall sup \tag{3.40}$$

The total cost of transport on the objective function will be given by Eq.(3.41):

$$CTTT = \sum_{sup} CTT_{sup} \tag{3.41}$$

3.2.3 *Main objective function*

The model developed to represent the production of a powder detergent is optimized using a simplified profit (Eq.(3.42)) as the main objective function.

$$\begin{split} Profit = \sum_{ye,j} priceprod_j \cdot \left(\sum_{l} y_{ye,l,j} + \sum_{i} z_{ye,i,j} \right) - \\ \sum_{ye,i,sup} CostP_{ye,i,sup} \cdot ccp_{ye,i,sup} - CTTT - \sum_{l} c_{pool_l} \cdot \sum_{ye,l,j} y_{ye,l,j} \end{split} \tag{3.42}$$

Note that only the variable cost of the intermediate tanks will be considered and not the fixed cost, unlike the objective function in Martín and Martínez, 2013. Analyzing the work of these authors, intermediate pools were not chosen in any of the cases studied, so it is assumed that in the cases considered in this study, they will not be selected either. However, for the sake of maintaining a general formulation, the possibility remains that these can be chosen but only considering variable cost. In this way, if the tanks are not selected considering the variable cost, it is demonstrated that neither would be considering also the fixed cost. In the case that any of the intermediate tanks is chosen, it would be necessary to reformulate the model to include the fixed costs. The reason for this simplification is to avoid including binary variables associated with the fixed cost, which complicates the problem computationally.

In addition, the ϵ-constraint method is used to include the environmental objective given as the carbon footprint allowed per year in the overall process. Thus, for each value of carbon footprint, a maximum profit will be obtained, being able to draw the Pareto curve that allows evaluating the problem as a multi-objective one. Note that a third objective is given by the detergent performance that must be achieved so that it is accepted by the consumer.

3.2.4 *Alternative formulation*

The large problem due to the number of ingredients, including suppliers and the price reduction policies results in a computational challenge. For a representative case of study, the previous formulation could not find a solution after days of computation. An alternative formulation is developed to make it tractable by eliminating the binary variables, using only continuous variables. The variable corresponding to the raw material flow ($ccp_{ye,i,sup}$) is reformulated to include an additional dimension to account for the discount policy ($ccp_{ye,i,sup,po}$).

In this way, the binaries that were used to select the best policy for each case can be removed at the expense of a larger number of equations. In the reformulation, this variable will be responsible for selecting and indicating which is the best policy through its indexes, similarly as it was formulated for the suppliers. For each year and for each raw material, the variable $ccp_{ye,i,sup,po}$ will select the supplier or suppliers, as well as the policy, through the amount purchased of raw material 'i' from each supplier and using each policy. The information provided by $ccp_{ye,i,sup,po}$ will be the amount purchased of raw material 'i' in the year 'ye' and from supplier 'sup' using policy 'po'. In short, its value corresponds to the amount purchased and its subscripts to the optimal suppliers and policies. This variable is schematically explained in Figure 3.1.

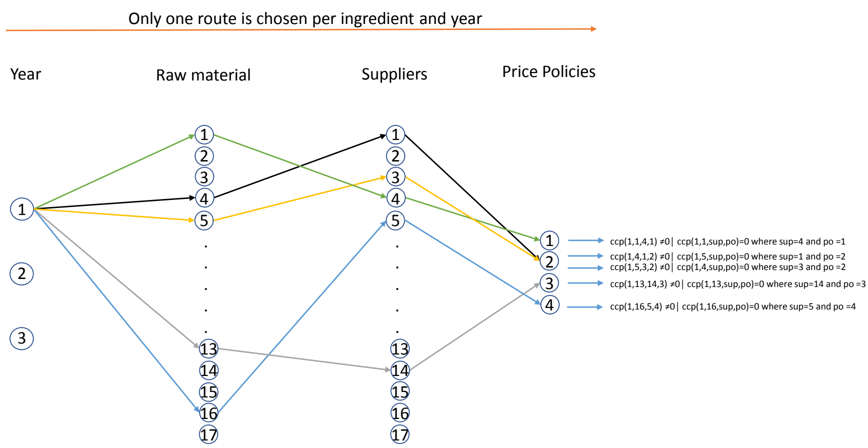

Figure 3.1: Example of the optimal selection of raw material, suppliers and price policies using $ccp_{ye,i,sup,po}$.

The introduction of a new dimension of $ccp_{ye,i,sup,po}$ modifies the model formulation. Eqs. (3.1),(3.26),(3.30),(3.31),(3.32),(3.40),(3.42) change in the new formulation. The new equations would be (3.43),(3.44),(3.45),(3.46),(3.47),(3.48),(3.49) as follows:

$$\sum_{po} ccp_{ye,i,sup,po} = \sum_{l} x_{ye,i,l} + \sum_{j} z_{ye,i,j} \forall ye, i, sup \tag{3.43}$$

$$Emision\ T_{ye,sup} = EmisionU_{sup} \cdot \sum_{i,po} ccp_{ye,i,sup,po} \forall ye, sup \tag{3.44}$$

$$costj_{ye,i,sup,1} = c0_{i,sup} - \left(\frac{c0_{i,sup} \cdot discount}{Lsup_{i,sup} - Linf_{i,sup}} \right) (ccp_{ye,i,sup,1} - Linf_{i,sup}) \forall ye, i, sup \tag{3.45}$$

$$costj_{ye,i,sup,2} = c0_{i,sup} \cdot \left(\frac{1}{1 + disct} \right) + c0_{i,sup} \cdot \left(\frac{\left(\exp\left(-\left(\left(\frac{1}{Lsup_{i,sup}}\right) + \left(\frac{10}{Lsup_{i,sup}}\right) \cdot ccp_{ye,i,sup,2}\right)\right)\right)}{\left(disct + \exp\left(-\left(\left(\frac{1}{Lsup_{i,sup}}\right) + \left(\frac{10}{Lsup_{i,sup}}\right) \cdot ccp_{ye,i,sup,2}\right)\right)\right)} \right) \forall ye, i, sup \tag{3.46}$$

$$Costj_{ye,i,sup,3} = c0_{i,sup} \cdot \left(ccp_{ye,i,sup,3} \right)^{\left(-powd_{i,sup}\right)} \quad \forall ye, i, sup \tag{3.47}$$

$$CTT_{sup} = CtransU_{sup} \cdot \sum_{i,po,ye} ccp_{ye,i,sup,po} \forall ye, i, sup \tag{3.48}$$

$$Profit = \sum_{ye,l} priceprod_j \cdot \left(\sum_{l} y_{ye,l,j} + \sum_{i} z_{ye,i,j} \right) - \sum_{ye,i,sup} CostP_{ye,i,sup} \cdot ccp_{ye,i,sup} - CTTT - \sum_{l} c_p ool_l \cdot \sum_{ye,l,j} y_{ye,l,j} \tag{3.49}$$

However, as discussed above, the problem is a multiperiod one, that is, not only one production period, one year, will be considered, but several years with different demands from the customers. This means that the price discount will be calculated each year, but the contracts will be made for several years. Therefore, if the first year a specific policy is chosen, the next one will have to use the same policy. Because binaries are not used, it will be necessary to introduce a penalty for configurations that do not choose the same policy every year. The same applies to suppliers, so that the same supplier is chosen every year. Thus, a penalty will also have to be introduced. Both the penalty for different policies and that for different suppliers can be calculated together introducing into the model the variable $\text{penalty}_{ye,i,sup,po}$. It is defined for each of the 3 years, Eqs.(3.50)-(3.52).

Year 1:

$$penalty_{1,i,sup,po} = \sum_{po}\sum_{sup} ccp_{1,i,sup,po} - ccp_{1,i,sup,po} \tag{3.50}$$

Year 2:

$$\begin{aligned} penalty_{2,i,sup,po} = \sum_{po}\sum_{sup} ccp_{1,i,sup,po} + \sum_{po}\sum_{sup} ccp_{2,i,sup,po} - \\ ccp_{1,i,sup,po} - ccp_{2,i,sup,po} \end{aligned} \tag{3.51}$$

Year 3:

$$\begin{aligned} penalty_{3,i,prov,po} = \sum_{po}\sum_{sup} ccp_{1,i,sup,po} + \sum_{po}\sum_{sup} ccp_{2,i,sup,po} + \\ \sum_{po}\sum_{sup} ccp_{3,i,sup,po} - ccp_{1,i,sup,po} - ccp_{2,i,sup,po} - ccp_{3,i,sup,po} \end{aligned} \tag{3.52}$$

With this formulation, for the cases in which the same supplier and the same policy are chosen over the 3 years (that is, the three-year contract with the same supplier is fulfilled) this penalty will be 0. This formulation also allows changing supplier and policy year after year if that is the management will. Therefore, Eqs.(3.34) and (3.37) are also affected giving rise to Eqs.(3.53) and (3.54).

$$Cost_{ye,i,sup,po} = Costj_{ye,i,sup,po} + penalty_{ye,i,sup,po} \;\forall ye, i, sup, po \tag{3.53}$$

$$CostP_{ye,i,sup,po} = cost_{ye,i,sup,po} + Costjf + penalty_{ye,i,sup,po} \forall ye, i, sup, po \tag{3.54}$$

3.3 CASE OF STUDY

To show the use of the formulation for the design of formulated products, a case study in Europe is considered. A number of suppliers per ingredient is taking into account. The facility that produces the three types of detergents is already installed and in operation.

It is assumed that bulk chemicals are subjected to market variability, such as surfactants, polymers and antifoam, and three price levels, low, medium and high, are used, while specialty chemicals price is fixed by contracts, for instance enzymes. The data used to apply the formulation to this case study can be found in Tables A.1-A.14 in the supplementary information. We divide this section to present the features commented on these lines starting with the definition of the suppliers.

3.3.1 *Suppliers*

Suppliers will be grouped by the type of chemical they supply:

- Inorganic Suppliers (from 1 to 3): They will be responsible for supplying fillers, builders and bleaches. Three suppliers will be considered with the same availability of raw materials and different prices depending on their proximity. The more expensive is the one that is closer to the manufacturing site and the cheapest is the one that is further away from it. This is so, because it would not make sense from the economic point of view to select a supplier that is more expensive and, at the same time, is further away since it is negative for both objectives (economic and environmental) and would never be selected.
- Organic suppliers (from 4 to 6): They will be responsible for supplying surfactants, polymers and antifoams. Three suppliers will be considered.
- Enzyme suppliers (From 7 to 12): They will be in charge of supplying the different enzymes used to eliminate specific stains. Six suppliers will be considered (two for each type of enzyme).

The optimal selection of suppliers is paramount since the distance affects both the price of the products and the environmental impact. It is interesting to consider different combinations of suppliers and analyze the effect on the formulation of the final product.

The main plants from three of the larger chemicals producers in Europe have been selected to be the suppliers on our detergent plant, which has been located in Frankfurt (Germany). In Figure 3.2, the relative location of the suppliers with respect to the plant is presented. The distances between the plant and suppliers will be included in the supplementary information.

3.3.2 *Prices of the raw material*

3.3.2.1 *Prices fixed with contracts*

The prices without applying the discounts, base prices, are indicated in the supplementary information. The discount policy selected will be applied to reduce the base prices based on the amount purchased, the discount parameters and the supplier. We set the discount parameters of the different policies to take the following values:

- discount = 0.5

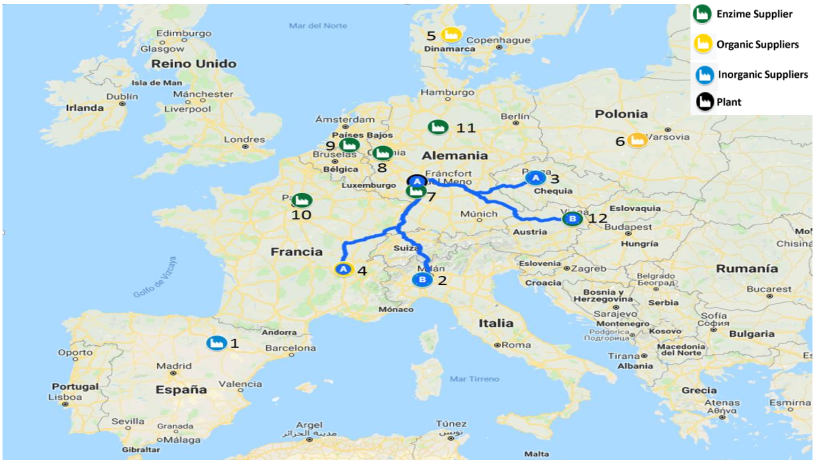

Figure 3.2: Location of the suppliers.

- disct = 1
- fixdisc = 0.15

In this case, the parameters have been adjusted randomly, while in a real problem, these parameters can be negotiated with the different suppliers. It is considered that the maximum discount will be 50%.

3.3.2.2 *Prices with variability*

It has been considered that the ingredients most susceptible to changes in their price throughout the year are surfactants, antifoams and polymers. Three different prices have been established for each ingredient, low, medium and high. The values are included in the supplementary information. This information is used to calculate the average price (see Section 3.2.2.7).

3.3.3 *Additional considerations*

The aim of this work is to develop a mathematical formulation for the design of formulated products. It is a multi-objective and multi-period problem that yields the composition of the final product as a function of the environmental impact. The economic benefit decreases when more environmentally friendly products are designed. A trade-off between both objectives is computed. To do this, in order to facilitate the location of this point, the maximum and minimum demand of the 3 years contract is assumed to be the same. Because if this is not the case, the model could spread the environmental impact among the different years, increasing the number of variables with which the program can work and making it difficult to analyze the results.

3.4 RESULTS

The problem of the design of three different powder detergents is formulated as a multi-objective, multi-period and multi-scale one. The solution to this problem should yield the selection of the supplier, the amount produced, and the ingredients selected subject to process and availability constraints. The main objective is the optimization of the profit for an allowed level of CO 2 emissions. Two formulations are developed. The first one consists of an MINLP of 5195 equations and 4320 variables (780 binary variables). The second one uses only continuous variables (NLP) with 11971 equations and 14083 variables. Although the MINLP model is much smaller in terms of equations and variables, the presence of integer variables makes it much more difficult to solve, so that a solution is not found in 20 h. Therefore, we evaluate the performance of the NLP model giving feasible results in the 20 h established as a limit with a tolerance lower than 6%. A commercial solver BARON is used for in an Intel Core i7–7700 computer with 3.6 GHz of speed and 32 Gb of RAM. Note the other global solvers such as GlOMIQO or ANTIGONE can also be used.

3.4.1 *Optimal selection of supplier, ingredients and pricing policies*

3.4.1.1 *Optimal economic solution*

The first result to be presented is the optimal economic product design. To compute it, the environmental impact will not be considered. Table 3.2 shows the selection of suppliers and the ingredients purchased.

Table 3.2: Results without environmental constraint.

Ingredients	Supplier	Amount(ton/year)	Optimal formulation (t_{ingre}/t_{prod})			Policy	HC (tCO2e/year)	Profit(M)
			A	B	C			
LAS	4	120	15%	15%	15%	-	1404	7.9529
ZEO	3	427	56%	50%	60%	2		
S.PERBO	1	95.5	5%	19%	5%	2		
S.SO	3	80	10%	10%	10%	3		
ANTI	4	0.8	0%	0%	0%	-		
CELL	12	12.67	3%	1%	1%	2		
CMC	4	0.8	0%	0%	0%	-		
WATER	13	63.37	12%	5%	8%	-		

The cheapest and most polluting ingredients have been selected. However, note that in some cases the farthest supplier has been selected (as in the case of ingredient S.PERBO and CELL) while in other cases the solution selects the closest one (such as the cases of LAS, ZEO, S.SO, ANTI and CMC). The reason behind is the fact the transportation cost of these ingredients is significant compared to the ingredient cost. Although the environmental impact is not being evaluated, it may not be profitable in some cases to buy ingredients from nearby suppliers because their cost is higher than the sum of their cost and that of transportation. Note that the suppliers selected are either the nearest or the most distant ones, but not the intermediate cases. This is the trade-off between ingredient and transportation cost. Extreme cases occur since the intermediate is not the best trade-off for that ingredient. In the case of water, its cost has not been considered as it is necessary and irreplaceable by another. Supplier 13 has a distance 0 (and therefore cost 0) because it is understood water is taken at the manufacturing site, unless, in the place where the plant is built, it will simply be necessary to connect it to the water network.

3.4.1.2 *Environmentally friendly product design*

The ϵ-constraint method will be used to include the second objective into the formulation. The selection of ingredients and suppliers will be evaluated aiming at maintaining the maximum profit. In this way, the ability of the system to adapt to more restrictive environmental policies is evaluated and, for an equivalent CO_2 value, how it is possible to modify the product composition to maintain the profit without significant variation. This study starts with a carbon footprint value of 1404 tCO_2 per year. Representing the Pareto curve of the profit versus the carbon footprint, Figure 3.3 is obtained.

It can be seen that the system has a high capacity to reduce the carbon footprint before a significant reduction of the profit occurs. By means of different configurations of ingredients/suppliers it is possible to reduce the CO 2 equivalent emitted to the atmosphere from 1404 tCO_2 e/year down to 850 tCO 2 e/year, representing a 40% reduction and, even though, the profit only decreases by 1.29%. As environmental impact decreases further along the Pareto optimality curve, the profit decreases sharply. There are no feasible solutions which show an environmental impact below 775 $tCO_{2e/year}$, since demands cannot be satisfied at that level of emissions. Part of the reason is that the environmental impact is an extensive variable that also increases with the volume of product. From 850 $tCO_2 e/year$ and 950 $tCO_{2e/year}$ it can be seen a rapid decrease of the profit and therefore this is the region for the optimal solution as it will be presented below.

The results of the selection of suppliers and the ingredients purchased as well as the composition of the different products are shown in Table

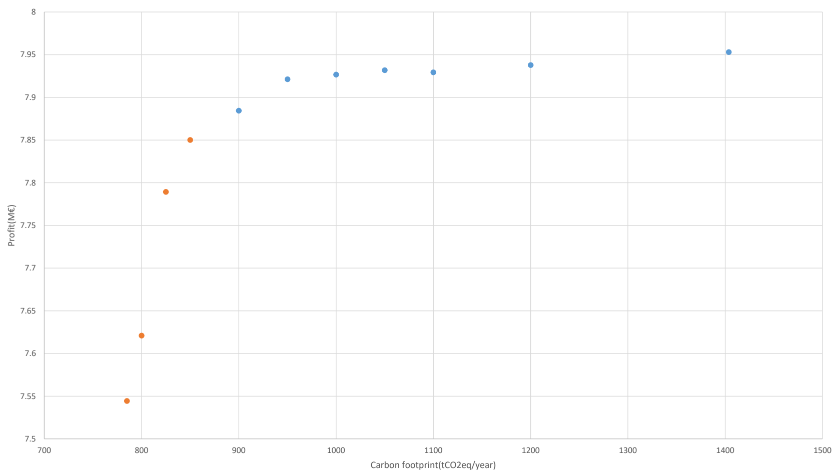

Figure 3.3: Pareto curve for the design of formulated powder detergents.

3.3 and 3.4. If the case of 950 $tCO_2e/year$ is compared with the case with no environmental constraints, it can be observed that the model is forced to choose less polluting ingredients, changing LAS by AE, ZEO by STPP and S.SO by X.SU. In all cases, these ingredients are less polluting but more expensive. With this composition, the facility can still maintain a benefit close to the maximum. This is achieved with an adjustment of the detergent composition. However, if a 785 $tCO_2e/year$ limit is established, the profit decreases considerably, reducing the profit by 3.9% when the carbon footprint decreases by 7.6% (from 850 $tCO_2e/year$ to 785$tCO_2e/year$) while between 1404 $tCO_2e/year$ and 850 $tCO_2e/year$ (40% reduction) the profit only falls by 1.3%. In this way, it is shown that the system loses the ability to compensate for the environmental impact when the carbon footprint value allowed is quite low. If the case of the carbon footprint of 850 $tCO_2e/year$ is compared with that of 950, 900 and 825 $tCO_2e/year$, the following changes can be observed:

- Comparing the cases of 950 $tCO_2e/year$ and 900 $tCO_2e/year$, it can be seen that the amount of builder decreases (less amount of STPP) and the amount of bleaches increases (larger amount of S. PERBO). Since bleaches are more expensive than builders, the cost of the raw materials increases. These changes in the composition of the final product are due to the fact that the bleaches have less associated carbon footprint than the builders and therefore, when the CO_2 emissions allowed are lower, the composition is to be altered to simultaneously meet the performance and the environmental constraints. If the comparison is made between the emission values of 900 $tCO_2e/year$ and 850 $tCO_2e/year$, something similar occurs. In this case, the purchase of STPP is further reduced, since the environmental limit is tighter, and the amount of X.SU is increased, which is more expensive. However, the most important change occurs in the group of polymers. The amount of polymers purchased goes from 0.8 t to 14.52 t per year to meet the performance constraint. Polymers are the most expensive substances after enzymes, so the change is significant. Finally, when comparing the cases of $850tCO_2e/year$ and $825tCO_2e/year$, it is observed that the amount of polymers necessary to reach the expected yields is doubled again, going up to 40 t per year. This is because the amount purchased of STPP and enzymes is reduced and therefore, raw materials cost rises again. Below $825tCO_2e/year$, the maximum demand cannot be met because combinations of ingredients that simultaneously meet the requirements of carbon footprint and performance cannot be found, so that by lowering the amount sold, the profit obtained falls.

- Regarding transportation, among the four cases considered (950, 900, 850 and 825 $tCO_2e/year$) the suppliers selected are usually the same. In most cases, the supplier is the one closer to the factory, except in the case of bleaches (S. PERBO and S. PERCA). For this type of ingredient, the supplier changes from supplier 1 (the farthest from the factory) in the case of $950tCO_2e/year$ to supplier 2 (intermediate supplier) in the case of 825 $tCO\ _2e/year$. Similarly, for X.SU the supplier changes from 3 to 1 and back to 2.

- The detergent composition is shown in Table 3.3. As the CO_2 emissions are to be smaller, the surfactant compositions decrease while the bleaches, the fillets and polymers increase. Typically, to improve the performance, a higher concentration of enzyme is used.

Therefore, the limit value of carbon footprint that best balances both objectives (economic and environmental) is the value of 850 t $CO\ _2$e/year since, below this value, the benefit begins to decrease abruptly with small variations in the limit of environmental impact and above that value, the benefit does not increase that much. For this limit value of carbon footprint, the map of the suppliers is showed in Figure 3.4.

Table 3.3: Optimal formulation with environmental impact constraints HC: 950, 900, 850 and 825 $tCO_2e/year$

	Optimal formulation(ti/tp) · 100							
HC	950 tCO2e/year							
Ingredients/ Products	AE	STPP	S.PERCA	X.SU	ANTI	CELL	CMC	WATER
A	15.00%	55.59%	5.00%	10.00%	0.10%	2.56%	0.10%	11.65%
B	15.00%	37.87%	24.28%	10.00%	0.10%	1.00%	0.10%	11.65%
C	15.00%	40.53%	22.13%	10.00%	0.10%	0.50%	0.10%	11.65%
HC	900 tCO2e/year							
Ingredients/Products	AE	STPP	S.PERBO	X.SU	ANTI	PRO	POLI	WATER
A	15.00%	36.31%	25.00%	10.00%	0.10%	1.84%	0.10%	11.65%
B	15.00%	37.18%	25.00%	10.00%	0.10%	0.97%	0.10%	11.65%
C	15.00%	37.76%	25.00%	9.67%	0.10%	0.40%	0.10%	11.65%
HC	850 tCO2e/year							
Ingredients/Products	AE	STPP	S.PERBO	X.SU	ANTI	PRO	POLI	WATER
A	15.00%	31.07%	25.00%	25.10%	0.10%	1.99%	0.10%	1.63%
B	15.00%	28.72%	25.00%	24.94%	0.10%	0.97%	3.53%	1.74%
C	15.00%	32.58%	25.00%	24.92%	0.10%	0.54%	0.10%	1.75%
HC	825 tCO2e/year							
Ingredients/Porducts	AE	STPP	S.PERBO	X.SU	ANTI	CELL	POLI	WATER
A	15.00%	26.42%	25.00%	25.03%	0.10%	1.78%	5.00%	1.68%
B	15.00%	26.42%	25.00%	25.03%	0.10%	1.78%	5.00%	1.68%
C	15.00%	26.42%	25.00%	25.03%	0.10%	1.78%	5.00%	1.68%

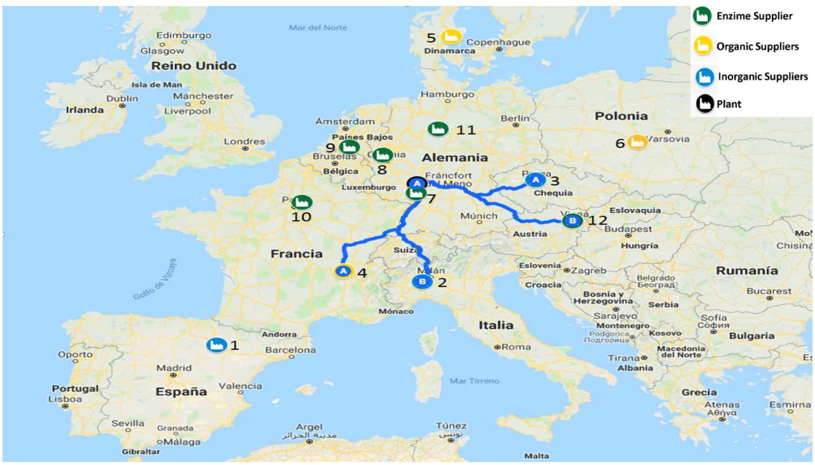

Figure 3.4: Selected suppliers to the optimal case.

Most of the ingredients that are purchased through contracts are abundant and policies 1, 2, 3 are used(see Table 3.4).

It is important to indicate that the upper limit of enzyme supplies is 20 tons per year, therefore, if the amount purchased is close to half of the available amount of enzyme, then policy 4 is not suggested. Therefore, in none of the cases raised, policy 4 is chosen. The selection of price reduction policies is complex from the computational point of view since the discount is very similar in all (except for 4). This fact is found in this work, but it can

Table 3.4: Results with environmental impact constraints HC: 950, 900, 850 and 825 tCO_2e/year.

HC ($tCO_2e/year$)	Ingredient	Amount(t/year)	Supplier	Price policy	Profit(M)
950	AE	120.00	4		7.921
	STPP	358.80	3	2	
	S.PERCA	134.25	1	2	
	X.SU	80.00	3	2	
	ANTI	0.80	4	-	
	CELL	12.18	12	2	
	CMC	0.80	4	-	
	WATER	93.18	13		
900	AE	120.00	4		7.884
	STPP	295.40	3	2	
	S.PERBO	200.00	2	2	
	X.SU	79.27	1	1	
	ANTI	0.80	5	-	
	PRO	9.82	12	2	
	POLI	0.80	4	-	
	WATER	93.18	13		
850	AE	120.00	4	-	7.85
	STPP	240.685	3	1	
	S.PERBO	200.00	2	2	
	X.SU	200.00	3	2	
	ANTI	0.80	4	-	
	PRO	10.41	12	2	
	POLI	14.52	4	-	
	WATER	13.58		-	
825	AE	119.89	4	-	7.789
	STPP	216.00	3	3	
	S.PERBO	199.77	2	1	
	X.SU	200.00	3	1	
	ANTI	0.80	4	-	
	CELL	9.29	12	2	
	POLI	40.00	4	-	
	WATER	13.41	13	-	

be different if the parameters of discounts change, which are established by negotiation with the different suppliers. For this reason, it is convenient not to discard any of it in the mathematical formulation.

3.5 CONCLUSION AND FUTURE WORK

In this work, we have developed a mathematical formulation for the optimal design of formulated products selecting the supplier and the ingredients to obtain three different types of detergents. This framework can be applied to any formulated product in the food, pharmaceutical and cosmetics industries among others. The results show that the proper selection of ingredients and suppliers allows a substantial reduction of the environmental impact, more than 40%, without significantly affecting the benefit. The simultaneous selection of suppliers, ingredients and discount policies provides the ability to adapt to different environmental limits. This work shows that the integrated product and process design and suppliers selection allows finding a trade-off between the benefit and significant reductions in environmental impact. However, there is a limit value beyond which the profit decreases sharply since it is no longer possible to compensate for the environmental impact without reducing the production or having to use more expensive ingredients which reduce the benefit.

Future work will seek to integrate this model within a supply chain, so as to also take into account different possible locations of the plant depending on the suppliers and also the customers. It is also possible to introduce different types of uncertainties (in customer demand for example) or other types of metrics, such as customer acceptance. This integrated problem will require additional analysis and solution procedures.

3.5.0.1 *Declaration of Competing Interest*

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

3.6 ACKNOWLEDGMENTS

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4

SIMULTANEOUS OPTIMIZATION OF THE DESIGN OF THE PRODUCT, PROCESS, AND SUPPLY CHAIN FOR FORMULATED PRODUCT

ABSTRACT

In this work, an integrated framework and a solution procedure are developed for the design of formulated products. The framework considers the design of the manufacturing process, the products, and supply chains simultaneously. The problem is a multi-period MINLP. A solution procedure consisting of two stages is developed. In stage 1, the model is initialized with the data provided by the market analysis and the optimal formulation for each product and for each location, individually. In stage 2, the model is optimized within the feasible region using the information from stage 1, and the amounts of raw material purchased from each supplier, product manufactured at each location, and product purchased by each customer are determined. The algorithm is used to evaluate the design of powder detergents in Europe, together with the location of the facilities, product composition, suppliers and price policies are selected.

Keywords: Supply chain ,Process and product design, Integrated problem, Formulated products

RESUMEN

En este trabajo se desarrolla un marco integrado y un procedimiento de solución para el diseño de productos formulados. El marco considera simultáneamente el diseño del proceso de fabricación, los productos y las cadenas de suministro. El problema es un MINLP multiperíodo. Se desarrolla un procedimiento de solución que consta de dos etapas. En la etapa 1, se inicializa el modelo con los datos proporcionados por el análisis de mercado y la formulación óptima para cada producto y para cada ubicación, individualmente. En la etapa 2, se optimiza el modelo dentro de la región factible utilizando la información de la etapa 1, y se determinan las cantidades de materia prima compradas a cada proveedor, el producto fabricado en cada ubicación y el producto comprado por cada cliente. El algoritmo se utiliza para evaluar el diseño de detergentes en polvo en Europa. Junto con la ubicación de las instalaciones, se seleccionan la composición del producto, los proveedores y las políticas de precios.

Palabras clave: Cadena de suministro, Proceso y diseño de productos, Problema integrado, Productos formulados,

4.1 INTRODUCTION

The market for consumer products is more competitive than ever as a result of globalization and increasingly demanding customers (Litster & Bogle, 2019). Customers do not only demand that a product meets their needs and likes (Tijskens & Schouten, 2014) but also personalized products, low lead time, quality improvements, sustainable and healthy products, and traceability. Therefore, for a new product to be competitive, it is not only necessary to adjust production costs, but also to comply with what is described above. The use of mathematical optimization techniques for the integrated design of processes and products is a powerful tool to screen among a large number of feasible products by considering only those that can be competitive (Taifouris et al., 2020a) and with a limited environmental impact (Martín & Martínez, 2013), so that resources and time are focused on a detailed design of the most promising products. This allows savings in development costs and reduces the time to launch new products. As a result, the process community has focused its attention on the integrated design of processes and products, with an increase in publications in recent years (Bernardo & Saraiva, 2005; Ng & Gani, 2018; uz Zaman et al., 2018). However, the supply chain has been studied in a subsequent stage. Integrating the design of the supply chain within the process and product design problem may result in more efficient products since it allows the centralization of production and promotes economies of scale (Tsay et al., 1999; Martín & Martínez, 2018). It also facilitates personalization in product design by considering the availability of raw materials and customer demands locally, increasing the flexibility of the entire process by achieving coordination between the three levels (product, process, and supply chain) (Marsillac & Roh, 2014). This coordination allows reducing lead times and improving customer service (Ellram et al., 2007). The integration of product, process, and supply chain design is addressed with the concept of three-dimensional concurrent engineering (3DCE) and, even though it is known since the beginning of 2000 (FINE, 2009), its practical application has been quite limited due to the complexity of the mathematical problem (Ellram et al., 2008; Caniato et al., 2012).

Formulated products are a type of complex products manufactured by mixing the ingredients so that the final product possesses specific physicochemical properties aligned with the needs and likes of its target customer (Audet et al., 2004). Its design depends on its formulation. As a result, the entire supply chain from the suppliers to the product that features the customer expectations, including the processing of the mixture across the manufacturing facility, has an impact on the selection of the process conditions and the different ingredients, (Martín & Martínez, 2013).

In formulated products, each different formula constitutes a new product, which facilitates its personalized design for different types of customers. Therefore, the integration of product, process, and supply chain design is especially important in these products. Currently, there is a limited number of scientific publications focused on the simultaneous design of processes and products, in the case of formulated products (Almeida-Rivera et al., 2007; Martín & Martínez, 2013; Zhang et al., 2017), some of them reach integrated supplier selection within the optimization model (Taifouris et al., 2020b), but do not integrate a complete supply chain. The integrated problem for the design of the product, process, and supply chain design is very difficult to address. On the one hand, pooling problems have bilinear products associated with mass balances (Misener et al., 2010), while the models to estimate the raw material prices are usually nonlinear (Audet et al., 2004). Besides, the models to estimate product quality, performance and process constraints are typically highly nonlinear equations, including bilinearities (Martín & Martínez, 2013). On the other hand, supply chains often have decision variables such as the location of the factories, the customers, as well as the suppliers of raw materials (Yue & You, 2014). These variables are binary variables, transforming the integrated problem into a large non-convex mixed-integer nonlinear programming (MINLP) model. Therefore, models that optimize supply chains usually have the production process and product design fixed, focusing on the analysis of the logistics. In these cases, the models to be solved are usually mixed integer-linear models (MILP) (Allaoui et al., 2018; Zahiri et al., 2018; Liu et al., 2020). Beyond a certain model size, commercial solvers cannot solve this type of problem and the development of specific algorithms for each problem is usually necessary. These algorithms can be genetic algorithms (Lin et al., 2009), algorithms based on linear relaxations (Thanh et al., 2010; Yue & You, 2014), or on decompositions, such as the Benders (Sahinidis & Grossmann, 1991) and Lagrange (Trespalacios & Grossmann, 2016) decompositions. However, no cases of application of these algorithms have been found in the integrated design of products, processes, and supply chains for the design of formulated products.

In this work, an optimization framework has been developed to address the integrated process, product, supply chain designs problem. It has been applied for the optimized design of a specific formulated product, detergent powder at a continental scale. The mathematical model to be optimized is a large non-convex MINLP whose solution is approached by developing a decomposition algorithm. The framework and the algorithm are general and flexible aiming at its use beyond the case study for large-scale problems. The rest of the paper is organized as follows. In Section 4.2, the mathematical optimization model is developed including the description of the problem, the supply chain integration into the reference work, and the development of the algorithm. In Section 4.3, the model is applied to a case study in Europe. In Section 4.4, the results are shown and in Section 4.5, the conclusions are discussed.

4.2 MATHEMATICAL MODEL

4.2.1 *Description of the problem*

The problem we address in this work is the simultaneous product, process, and supply chain design for a specific type of formulated product, detergent powder. The objective is to develop a mathematical model and a decomposition algorithm that allow us to optimize not only the formulation of the product and the operating conditions of the plant but also the location of these plants, the selection of the best ingredients and suppliers, as well as the amount sold to each customer.

We use the work of Taifouris et al., 2020b as a starting point and refer the reader to that work regarding the details on the modelling of the process constraints, the product performance, and the price policies for the ingredients. The final product consists of a formulated material within the family of consumer products, detergent powder. This is obtained by mixing up to 14 different ingredients, classified into 8 groups. The ingredients, their abbreviations, and their carbon footprints (HC) are shown in Table 4.1.

Table 4.1: List of considered ingredients and their associated environmental impact

Group	Ingredient	Abbreviation	HC (tCO2/tk)
Surfactant	Linear alkyl aryl sulfonates	LAS	4.2
	Alcohol ethoxylates and alkyl amides	AE	3.7
Builder	Polyphosphates	STPP	1.014
	Zeolite	ZEO	1.76
Bleach	Sodium perborate tetrahydrate	S. PERBO	0.4
	Sodium percarbonate.	S. PERCA	0.4
Fillers	Sodium sulfate	S.SU	0.3
	Xylene sulphonate	X.SU	0.03
Antifoaming agents	-	ANTI	1.76
Enzymes	Protease	PRO	3.69
	Lipase	LIP	3.69
Polymers	Sodium polyacrylate	S. POLY	0.02
	Polyethylene glycol	POLYGLY	0.17
Water	Water	WAT	0

In each group, the ingredients differ by their price and their environmental impact. Several suppliers are considered for each ingredient depending on their nature whether they are organic, inorganic, or enzymes. The distances between suppliers and factories are calculated and evaluated from an economic point of view. The price of some of the ingredients (i.e. builders, bleaches, fillers, and enzymes) is considered fixed throughout the year by a contract, selecting the best price policy (linear, exponential, constant elasticity and fixed) based on the amount used of them in the production, while the price of the other ingredients (i.e. surfactant, antifoaming agents, and polymers) may vary throughout the year, due to market fluctuations.

During the production process, which mainly consists of ingredients mixing, slurry drying, and the addition of additives, the different units must operate under certain conditions so that the production of the final product is feasible and its performance meets the consumer needs. Therefore, it is necessary to introduce a series of constraints. Due to confidentiality issues, the ones selected based on open literature were the particle size and cake strength of the final product. Three different types of products are produced with different prices and performances. In this way, a larger market spectrum can be addressed. To characterize the three products, the performance of each one is added in the model as a constraint, setting the maximum and minimum values for each product. In addition, the model is multi-period because the contracts with the suppliers are multiannual. We consider two years as the time horizon.

The objective of this work is to add the dimension of the supply chain to the problem formulated by Martín and Martínez, 2013 and Taifouris et al., 2020b, to provide information on the ingredients and detergent composition, the selection of suppliers, price policies, and the location of the production facilities from an economic point of view. This type of model is characterized by its large size and mathematical complexity, having a large number of nonlinear equations and bilinear products. This makes it quite difficult to solve this type of problem directly using a commercial solver. The size and complexity of the problem, especially for supply chains at the continental scale, require the development of a methodology that allows solving the problem considering the entire problem of the detergent production that is, the product, process, and supply chain simultaneously.

4.2.2 *Supply chain design*

For the sake of the length of the manuscript, we refer readers to previous work for the models regarding the process and product constraints. In this work, we only indicate how the supply chain is added as well as the development of the algorithm to address its solution. The basic model was presented in Taifouris et al., 2020b. Building on that formulation, see also the supplementary material, the dimension of the supply chain is added. This requires the addition of a new dimension to many variables, the location (loc). The modified variables are shown in Table 4.2. In addition, it is necessary to add new variables and parameters. In addition, the variable $cv_{ye,j,cli,loc}$ is defined to represent the amount of the product 'j' sold to the customer 'cli' by the factory located at location 'loc' in the year 'ye'. This variable is included in the objective function since, together with the price of the products, it represents the income obtained by each factory. The total income is calculated by Eq.(4.1).

$$Income = \sum_{ye,j,cli,loc} cv_{ye,j,cli,loc} \cdot priceproduct_j \tag{4.1}$$

Table 4.2: List of variables and parameters with location dimension

$x_{ye,i,l,loc}$	$costeing_{ye,i,sup,po,loc}$	$MassprodT_{j,loc}$
$y_{ye,l,j,loc}$	$CostP_{ye,i,sup,po,loc}$	$division_{ye,i,sup,po,loc}$
$z_{ye,i,j,loc}$	$Particle_{j,loc}$	$ccp_{ye,i,sup,po,loc}$
$p_{ye,l,k,loc}$	$Cakest_{j,loc}$	$CTT_{sup,loc}$
$PQ_{j,k,loc}$	$MassIng_{ye,i,sup,po,loc}$	$division_{ye,i,sup,po,loc}$
$cv_{ye,j,cli,loc}$	$Massprod_{ye,j,loc}$	$CtransU_{sup,loc}$
$distance_{sup,loc}$	$Ctrans_{sup,loc}$	$Performance_{j,loc}$

Where $priceproduct_j$ are the prices of the three products considered and their values are in the supplementary material. It is considered that the price of the products only depends on the quality perceived by the clients. The relationship between price and location is not considered directly since it can be indirectly related to purchasing power and perceived quality. Both depend on the location and set the demand for different products with different prices, affecting the price of the final product chosen. The introduction of this new variable implies the introduction of two new inequalities and one equality constraint so as to be able to meet the demand Eqs. (4.2),(4.3), and (4.4).

$$\sum_{loc} cv_{ye,j,cli,loc} \leq DemandMax_{ye,cli,j} \ \forall ye, j, cli \tag{4.2}$$

$$\sum_{loc} cv_{ye,j,cli,loc} \geq DemandMin_{ye,cli,j} \ \forall ye, j, cli \tag{4.3}$$

$$\sum_{cli} cv_{ye,j,cli,loc} = Massproduc_{ye,j,loc} \ \forall ye, j, loc \tag{4.4}$$

Where $\mathrm{DemandMax}_{ye,cli,j}$ and $\mathrm{DemandMin}_{ye,cli,j}$ are the maximum and minimum demand of the product 'j' by the client 'cli' in the year 'ye', respectively. $\mathrm{Massproduct}_{ye,j,loc}$ is the amount of the product 'j' that is produced in the location 'loc' in the year 'ye' and is defined by Eq.(4.5).

$$Massproduc_{ye,j,loc} = \sum_{l} y_{ye,l,j,loc} + \sum_{i} z_{ye,i,j,loc} \quad \forall ye, j, loc \tag{4.5}$$

Where $z_{ye,i,j,loc}$ and $y_{ye,l,j,loc}$ are the flows of material, see also the supplementary material for further details. The equation that determines the transportation costs from the suppliers to the factory has already been described in the work by Taifouris et al., 2020b. In this work, a similar strategy is followed to compute the transportation cost for the product sold to customers. First, the unit transport cost is calculated. For that, the cost of transportation from the production plant at location 'loc' to the customer 'cli' is determined. The price is calculated considering consumption of 25 L/100 km and a diesel cost of 1 €/L. Therefore, the price per kilometer is 0.25 €/km and the transport cost is calculated by Eq.(4.6).

$$CtransCli_{loc,cli} = distC_{loc,cli} \cdot 0.25€/km \ \forall loc, cli \tag{4.6}$$

Where $\mathrm{distC}_{loc,cli}$ is the distance between the location where the product is produced and the customer who buys them. The unit cost is given by Eq.(4.7).

$$CtransCliU_{loc,cli} = \frac{CtransCli_{loc,cli}}{LoadingCapacity} \ \forall loc, cli \tag{4.7}$$

Where the loading capacity of each truck is 7 t and the total cost of transportation is calculated by Eq.(4.8).

$$Total\,\mathrm{Cos}\,tTc = \sum_{ye,j,cli,loc} CtransCliU_{loc,cli} \cdot cv_{ye,j,cli,loc} \tag{4.8}$$

Border taxes, in the case of application, are included in the initial cost of raw materials ($co_{i,sup}$, see supplementary material), and in the price of the products ($\mathrm{priceproduct}_j$).

Finally, it is necessary to add the fixed cost (FixCost) to penalize the installation of a large number of small facilities. If this cost were not added, the mathematical optimization model would choose to build as many plants near the suppliers and customers as needed with the aim of reducing transportation costs. Fixcost is accounted for using a binary variable ($bi1_{loc}$) and added to the objective function. Therefore, the new objective function is given by Eq.(4.9).

$$\begin{aligned}profit = &\sum_{ye,j,cli,loc} cv_{ye,j,cli,loc} \cdot priceproduct_j - \\ &\sum_{ye,i,\mathrm{sup},po,loc} \mathrm{Cos}\,tP_{ye,i,\mathrm{sup},po,loc} \cdot ccp_{ye,i,\mathrm{sup},po,loc} - \\ &\sum_{l,loc} Cpool_l \cdot \sum_{ye,j} y_{ye,l,j,loc} - Total\,\mathrm{Cos}\,tTC - \\ &\sum_{ye,i,\mathrm{sup},po,loc} CtransS \cdot ccp_{ye,i,\mathrm{sup},po,loc} - \sum_{loc} bi1_{loc} \cdot Fix\,\mathrm{Cos}\,t_{loc}\end{aligned} \tag{4.9}$$

Another difference between the formulation of this work and that of Taifouris et al., 2020b is that it is necessary to calculate the distances between locations, suppliers, and customers. We use the coordinates to determine the distances between these three variables, using the Eqs. (4.10)-(4.14). The coordinates can be consulted in the supplementary information.

$$\Lambda lat = |lat1 - lat2| \cdot \frac{pi}{180} \tag{4.10}$$

$$\Lambda long = |long1 - long2| \cdot \frac{pi}{180} \tag{4.11}$$

$$a = \sin^2\left(\frac{\Lambda lat}{2}\right) + cos\left(lat1 \cdot \frac{pi}{180}\right) \cdot cos\left(lat2 \cdot \frac{pi}{180}\right) \cdot sin^2\left(\frac{\Lambda long}{2}\right) \tag{4.12}$$

$$c = 2 \cdot \arcsin\left(\sqrt{a}, \sqrt{(1-a)}\right) \tag{4.13}$$

$$D = R \cdot c \tag{4.14}$$

Where 'lat' is the latitude and 'long' is the longitude of the position of the supplier, location, or customer. D is distC $_{loc,cli}$ (km) or distance$_{sup,loc}$ (km) (depending on the coordinates used) and R is the radius of the Earth (6371 km). Note that in Taifouris et al., 2020b, the variable "distance" was a vector that only depended on the supplier, since one location alone was considered. However, in this work, this variable becomes a matrix that depends on the supplier and the location.

4.2.3 *Development of the algorithm linearization-solution*

With a new dimension added (locations) and the fact that the number of locations to be considered is expected to be large, the size of the formulated optimization problem becomes another complexity. In addition, the binary variables associated with the fixed cost (bi1$_{loc}$) transform the previous problem into a mixed integer nonlinear programming (MINLP) problem. As a result, the model cannot be solved directly using a commercial solver (i.e. DICOPT or BARON). Therefore, an algorithm is developed to address the problem. It consists of two stages, such as presented in fig: 4.1.

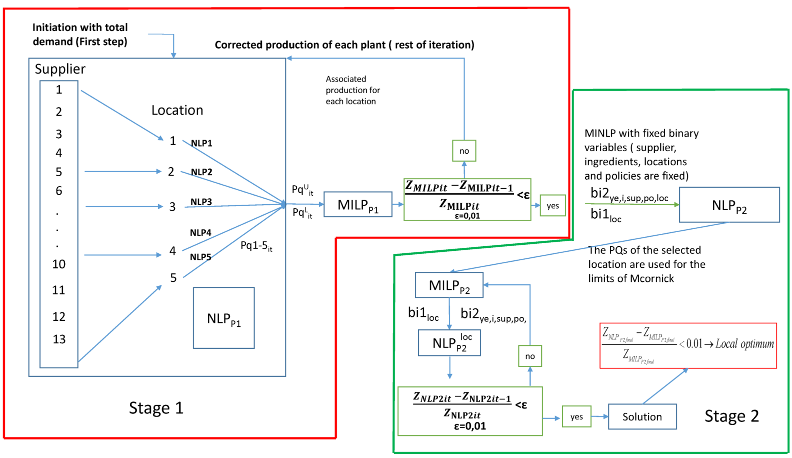

Figure 4.1: Example of application of the algorithm linearization-resolution.

In the first stage, the MINLP is linearized and transformed into a MILP $_{P1}$ using the results of the NLPs of each location (NLPs$_{P1}$). The MILP is solved using a commercial solver and its results are used to fix the decision variables (suppliers, ingredients, and pricing policies). This information is saved in a binary variable, bi2 $_{ye,i,sup,po,loc}$ and is used to transform the initial problem (MINLP) into an NLP (the '$bi1_{loc}$' binaries are also fixed by the MILP P1), passing to the second stage of the algorithm. In the second stage, a final solution is obtained. Note this new binary variable $bi2_{ye,i,sup,po,loc}$ was not in the original MINLP. They are generated in the linearized program (MILP $_{P1}$) to save the decision variables and send them to the global model (NLP $_{P2}$).

4.2.3.1 *Stage 1: linearization of the global problem (MINLP to MILP)*

The first stage consists of a linearization of the MINLP. The MINLP contains both nonlinear equations (i.e. price policies) and bilinear products (i.e. product performance equations, mass balances, etc.). To linearize the nonlinear equations, we apply piecewise linear approximations. The nonlinear equations correspond to the equations used to calculate the discount applied to the price of ingredients (see supplementary material and Taifouris et al., 2020b). These equations strongly depend on the upper and lower limits of raw material availability, so linearization cannot be applied using the same points in all ingredients since the linearization would not be adequate. Therefore, analyzing the nonlinear profiles, for each ingredient different linearization points are chosen, adjusting to the shape of the curves. To approximate the bilinear products, McCormick envelopes are used. Regarding McCormick envelopes, the proper selection of the upper and lower limits of the involved variables determines the accuracy of the approximation of the bilinear products. To compute these limits, the mathematical models developed in previous work are used. They correspond to the optimization considering a single location (each one of the NLP within NLP $_{P1}$ in Fig. 4.1), a single customer, and multiple suppliers for each type of ingredient. If we take into account the consideration that the optimal composition depends on the demand, the suppliers available for that factory, and local legislation, we can apply the NLPs developed in previous works to each of the locations considered in this work to obtain a first estimate of the optimal composition per location.

Since only one location is considered in each model NLP_{P1}, the number of equations is not larger than in previous works and therefore they can be solved to global optimality using a commercial solver. In addition, each model is independent of any other. Thus, they can be solved in parallel, so the total computational time corresponds to the solution time of a single NLP. After solving them, we can use this information to calculate the limits of the McCormick envelopes, considering that the correct value will be in a margin of 20% with respect to the value obtained from the NLPs, the limits are calculated by Eqs. (4.15) -(4.16). This value can be readjusted if needed.

$$PQ^L{}_{j,k,loc} = 0.9 \cdot PQ_{NLP1-68j,k} \forall j,k,loc \tag{4.15}$$

$$PQ^U{}_{j,k,loc} = 1.1 \cdot PQ_{NLP1-68j,k} \forall j,k,loc \tag{4.16}$$

Where PQ $^{U}_{j,k,loc}$ and PQ$^{L}_{j,k,loc}$ are the upper and lower limits of the McCormick envelopes, respectively. In order to initialize these NLP models, we need representative values of the demand per location to fix a maximum and minimum value of production. In the first iteration, we do not know the fraction of the total production that may be assigned to each location and therefore, the maximum and minimum total demand is fixed to each location. In this way, each NLP $_{P1}$ has the same demand. This is updated from the second iteration onwards. When the McCormick limits are established and the MILP $_{P1}$ is solved more realistic values for the demand are selected for each location, readjusting the optimal composition of the product in each NLP $_{P1}$ (in each location) and improving the estimation of the McCormick limits. Subsequently, this information is sent back to the MILP $_{P1}$ and new results are obtained, better than previous results. When the results of two iterations are within 1%, the iterative process stops, and the results are given as valid.

4.2.3.2 *Stage 2: Solution of the global model without linearization (NLP $_{P2}$)*

Once the MILP $_{P1}$ is solved, its results are used to set suppliers, ingredients, locations to build factories, and pricing policies in the original problem. In order to extract this information, it is necessary to add Eq.(4.17) to the MILP $_{P1}$ model.

$$ccp_{ye,i,\sup,po,loc} - bi2_{ye,i,\sup,po,loc} \cdot Lsub_{i,\sup} \leq 0 \quad \forall ye,i,\sup,po,loc \tag{4.17}$$

Therefore, if 'ccp' is different from zero, 'bi2' will be 1. As 'ccp' is only different from zero when the best suppliers, ingredients, locations, and policies are selected, 'bi2' will be 1 for that combination of suppliers, ingredients, locations, and policies. Due to the need for the use of binary variables, we add the Eq.(4.18) in the MILP$_{P1}$ to use the same price policy and supplier all years, and therefore, it is no longer necessary to include penalty functions to ensure that the same supplier and price policy are selected over the years. That was a particular reformulation needed in the previous work to avoid converting the optimization problem in an MINLP (Taifouris et al., 2020b).

$$bi2_{1,i,\text{sup},po,loc} = bi2_{2,i,\text{sup},po,loc} \quad \forall i, \text{sup}, po, loc \tag{4.18}$$

Besides, Eq.(4.19) is added to select only one pricing policy.

$$\sum_{po} bi2_{ye,i,sup,po,loc} \leq 1 \tag{4.19}$$

Eq.(4.20) is added to select locations, using 'bi1'.

$$bi2_{ye,i,sup,po,loc} - bi1_{loc} \leq 0 \tag{4.20}$$

It is necessary to remember that bi1 $_{loc}$ is introduced in the model to determine the fixed costs, as indicated in previous sections (see the objective function in Section 4.2.2). The binary variables can be used differently. If 'bi2' is fixed, 'ccp' can only be different from zero for the case in which 'bi2' is one. Therefore, the values of 'bi2' of MILP $_{P1}$ are added in the NLP $_{P2}$ using the Eq.(4.21).

$$ccp_{ye,i,\text{sup},po,loc} - bi2_{ye,i,\text{sup},po,loc} \cdot \text{Lsup}_{i,\text{sup}} \leq 0 \quad \forall ye, i, \text{sup}, po, loc \tag{4.21}$$

The fixed value for the binary 'bi1' is introduced in the objective function of the NLP $_{P2}$ to determine the fixed costs. Note both 'bi1' and 'bi2' are variables in the MILP $_{P1}$ and parameters in the NLP $_{P2}$. Since all binary variables are set by the MILP $_{P1}$, the initial MINLP is transformed into an NLP $_{P2}$ that let us find a solution in the feasible region of the problem. However, it should be noted that the global optimum cannot be guaranteed, but it is possible to solve the large integrated process product and supply chain design problems that cannot be addressed using a commercial solver directly.

Next, once the NLP $_{P2}$ has been solved, the results corresponding to the optimal formulation of the detergents, PQ are used as the next limits in the MILP $_{P2}$ model, transforming the problem in an iterative process that finishes when the difference between the result in the objective function of the NLP $_{P2}$ and the previous iteration is less than an ϵ value (see the Fig. 4.1). The only difference between MILP $_{P1}$ and MILP $_{P2}$ is that the McCormick envelope limits are set by NLP $_{P1}$ in the case of MILP $_{P1}$, while in the case of MILP $_{P2}$ are set by the results of NLP $_{P2}$.

4.3 CASE OF STUDY

The aim of this work is to optimize the design of the process, product, and supply chain simultaneously. We apply the methodology shown in Section 4.2 to the case of Europe. We consider 68 locations to build the factories and 29 possible suppliers corresponding to the major chemical companies in the continent. The demand considered for each customer is shown in Table 4.3.

Table 4.3: Demands of the costumers.

Demands							
	Product(t/ye)				Product(t/ye)		
Costumer	1	2	3	Costumer	1	2	3
1	100	20	5	8	50	25	5
2	10	100	15	9	100	10	5
3	5	100	10	10	150	15	5
4	2,5	50	15	11	50	5	5
5	5	100	10	12	25	100	10
6	100	50	5	13	10	25	100
7	15	50	15	14	100	25	5

Even though the different models integrated by the algorithm make it possible to establish different demands for each year, the same demand is established in order to facilitate the analysis of results and analyze the coherence of the results provided by the algorithm. Suppliers, locations, and customers can be seen in Fig. 4.2. The customers correspond to real locations of major retailers across Europe.

4.4 RESULTS

In this Section, the results of applying the algorithm developed in this work to the case study described in Section 4.3 are commented. On the one hand, the computational performance of the algorithm is discussed, indicating the computation time of each stage of the algorithm, the number of iterations necessary to solve the proposed problem and its comparison with commercial solvers. On the other hand, the results referring to the optimal selection of suppliers, locations, formulation, and customers are analyzed. The algorithm is executed in an Intel Core i7-7700 computer at

Figure 4.2: Locations, suppliers, and customers

3.6 GHz (4.2 GHz as turbo frequency), 65W of TDP, 4 core with 8 threads, and 32 Gb of RAM (1200 MHz).

4.4.1 *Computational performance of the algorithm*

In Table 4.4, the total CPU time of each stage and the number of iterations of each iterative process within each stage are shown, and this information is also compared with that of applying two commercial solvers (BARON and DICOPT).

Table 4.4: Computational results.

Stage	Problem size		Iteration number	Z		Time per iteration(s)	Total time(s)
1	NLPP1	Eqs= 12.573	1	-	-	500	1714
		Vars=16.876					
			2	-	-	500	
	MILPP1	Eqs=3.568.820	1	10846	-	706	
		Vars= 3.019.881(413)					
			2	10860	1.00E-03	8	
2	NLPP2	Eqs= 864,950	1	10829	-	170	358
		Vars= 882,247					
			2	10834	4.00E-04	172	
	MILPP2	Eqs=3.568.820	1	10861	-	9	
		Vars= 3.019.881(413)					
			2	10860	-	7	
Commercial Solvers							
BARON	Eqs= 1,236,069		-	No solution	-	-	72000
DICOPT	Vars=974,037(68)		-	Infeasible	-	-	6548

For the case study presented in this work, only the application of the algorithm has given any results. BARON was used to solve NLP p_1, CPLEX for the MILP's, and CONOPT for NLP p_2. In stage 1, 2 iterations were necessary to converge. The total computation time of stage 1 is 1714 seconds. Most of this time is used to solve NLP $_{P1}$ s that consume 500s of solution time for each iteration. With regards to stage 2, the second iteration provided a result similar to the one obtained in the first iteration. The iterative process does not improve the solution. This may be due to the solution provided by the NLP solver, CONOPT. Changing the limits of the McCormick envelopes with the information from the NLP $_{P2}$ does not significantly improve the solution in this specific case. Therefore, the total computation time of stage 2 is 358 s. The upper bound, provided by the relaxed problem (MILP) is 10860 while the lower bound (NLP $_{P2}$) is 10834. The difference is only 0.24%, giving as optimal results those obtained in the first iteration of stage 2. Note that we cannot ensure the global optimum. Global solvers (i.e BARON), due to the complexity and size of the case study presented, do not provide us with any results and even a local solver such as DICOPT does not provide us with a valid result either. Therefore, the result provided by the algorithm is taken as the only optimal value that can be calculated and it is evaluated if the result is logical with the location of the suppliers, the demands of the clients, the distribution of the production of the factories, and the selection of policies.

4.4.2 *Results of the case study*

While the MILP $_{P1}$ sets the decision variables, such as, which suppliers, ingredients, locations to build the factories and pricing policies to choose for each ingredient, the NLP $_{P2}$ sets the amounts of raw material purchased, the amount of product produced, the amount sold to each customer, and the formulation of detergents. Table 4.7 shows the purchased amount of the selected ingredients and Table 4.5 shows the total amount of each product produced by each location. Fig. 4.3 shows the locations chosen as optimal and the suppliers that supply the ingredients to the locations. As it can be seen in Table 4.7, the selected ingredients are the cheapest (see supplementary information) since environmental impact limits have not been established so that the results are easier to interpret and verify that the algorithm is working properly.

Each location centralizes the purchases of its ingredients in a single supplier by type of ingredient (organic, inorganic or enzymes) since they have enough raw material available. The centralization of purchases allows obtaining the maximum possible discount in the prices of the ingredients. In addition, the closest suppliers for each of the locations are chosen, reducing transport costs.

The optimal composition of each product in each selected location can be seen in Table 4.6. The optimal composition of the 3 products is very similar

Table 4.5: Total produced amount of each product by each location

	Production		
Product	A	B	C
1	75	1200	170
2	600	650	100
3	130	60	260

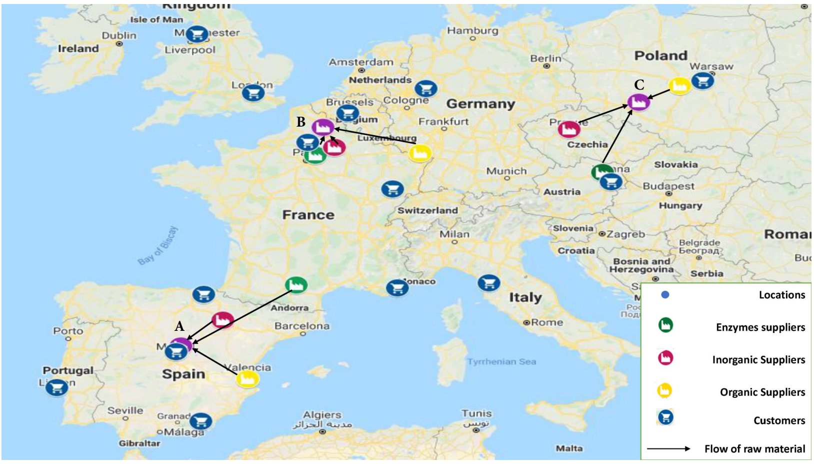

Figure 4.3: Locations, suppliers, and customers

in the 3 selected locations. Therefore, it is possible to refer to products 1, 2 and, 3 without loss of generality or specifying the factory that produces it. On the one hand, product 1 requires a larger fraction of enzymes in its composition (2.5 times higher) to meet its expected performance. On the other hand, product 2 has the same fraction of the enzyme as product 3, but its percentage of bleach is higher. It can be seen (In Eq.(B23).) of the supplementary information) that the bleaches have a very important effect on the washing performance and allow product 2 to have an intermediate performance between products 1 and 3 without having to increase its concentration in enzymes since these have a very high cost.

Table 4.6: Optimal composition of the products in each location.

	Optimal formulation%(tk/tp·100)								
Location	A								
Ingredients/	Surfactant	Builder	Bleach	Filler	Antifoam	Enzyme	Polymer		Water
Products	1	4	6	7	9	10	12	13	Water
1	15.00%	60.00%	5.00%	16.87%	0.10%	2.43%	0.00%	0.10%	0.50%
2	15.00%	50.00%	18.79%	10.00%	0.10%	1.00%	0.10%	0.10%	5.01%
3	15.00%	60.00%	5.41%	17.89%	0.10%	1.00%	0.10%	0.10%	0.50%
Location	B								
Ingredients/	Surfactant	Builder	Bleach	Filler	Antifoam	Enzyme	Polymer		Water
Products	1	4	6	7	9	10	12	13	Water
1	15.00%	55.51%	5.00%	21.23%	0.10%	2.56%	0.00%	0.10%	0.50%
2	15.00%	45.82%	20.68%	16.80%	0.10%	1.00%	0.10%	0.00%	0.50%
3	15.00%	60.00%	5.41%	17.89%	0.10%	1.00%	0.10%	0.00%	0.50}
Location	C								
Ingredients/	Surfactant	Builder	Bleach	Filler	Antifoam	Enzyme	Polymer		Water
Products	1	4	6	7	9	10	12	13	Water
1	15.00%	60.00%	5.00%	10.00%	0.10%	2.43%	0.00%	0.10%	7.37%
2	25.00%	48.16%	10.63%	10.00%	0.10%	1.00%	0.10%	0.00%	5.01%
3	15.46%	60.00%	5.00%	10.00%	0.10%	1.00%	0.10%	0.00%	8.34%

Regarding production, if the demands shown in Table 4.3 and the locations of the customers (see Fig. 4.2) are analyzed, it can be seen that the countries of central Europe demand a larger amount of the high-quality and high-price product (product 1), while Spain, Portugal and Italy demand lower-quality and lower-price products (product 2). Finally, the countries of Eastern Europe demand the lowest priced products (product 3). For this reason, the three factories installed have a different distribution of products in their production (see Table 4.5). The most manufactured product in each of them depends on the demand of customers close to them. Thus, the plant located in Spain shows a higher production of product 2, since the closest customers have a higher demand for this product. Similarly, it occurs with the factory located in France and Poland. Noted that the plant located in France is the one that produces the most, not only because it has more customers around it, but also because they are the ones that consume the most. Therefore, it is the one that produces the highest benefit. Thus, there is a centralization of production, being factory B the most prominent case. This allows reducing both the costs of raw materials (economy of scale) and the costs of distributing products. Regarding the price policies, we can see in Table 4.7 that all the ingredients are purchased using policies 2 and 3. Because both policies provide a very similar reduction in prices for the purchased amounts of ingredients, it is not possible to select the policy clearly between the two. However, policies 1 and 4 are not chosen in any case. In fact, if the raw material were purchased using policy 1 instead of policy 2 or 3, the cost of the raw material would be between 18-26% higher.

Table 4.7: Amount purchased of each ingredient by the selected supplier.

	Amount (t)				
Ingredient	Supplier	Policy	A	B	C
LAS	4	-	120.72	0.00	0.00
	11	-	0.00	286.50	0.00
	28	-	0.00	0.00	90.69
ZEO	3	2	423.02	0.00	0.00
	10	3	0.00	1000	0.00
	24	3	0.00	0.00	306.16
S.PERBO	10	2	0.00	197.66	0.00
S.PERCA	3	3	123.50	0.00	0.00
	24	3	0.00	0.00	32.13
S.SU	3	2	95.91	0.00	0.00
	10	3	0.00	374.40	0.00
	24	3	0.00	0.00	53.00
ANTI	4	-	0.81	0.00	0.00
	11	-	0.00	1.91	0.00
	28	-	0.00	0.00	0.53
PRO	6	3	9.12	0.00	0.00
	9	2	0.00	37.83	0.00
	25	3	0.00	0.00	7.73
S.POLY	4	-	0.73	0.00	0.00
	11	-	0.00	0.71	0.00
	28	-	0.00	0.00	0.36
POLYGLY	4	-	0.08	0.00	0.00
	11	-	0.00	1.20	0.00
	28	-	0.00	0.00	0.17
WAT	29	-	31.09	9.55	39.23

4.5 CONCLUSIONS

An algorithm has been developed for the integrated design of the process, product, and supply chain for formulated products. It consists of two stages. Stage 1 initializes the problem, providing the information for bounds and sets the decision variables. Stage 2 is responsible for product design and selection of the amount purchased for each ingredient from each supplier selected in Stage 1, the amount sold to each customer and the amount manufactured in each of the previously set locations.

From the results of this work, it can be concluded that for the integrated design of products, processes, and supply chains, it is necessary to adapt the problem in order to be solved. If the model is complex enough, commercial solvers cannot find a solution. After the development of an algorithm adapted to the particular case of detergent production in Europe, it was found that the algorithm could find an optimal solution (even though a global optimum could not be ensured) in less than an hour. After analyzing the results, the solution found was logical with the problem posed. It was decided to build 3 different factories, one focused on each type of product and each type of market to reduce the transportation costs of finished products. Purchases were centralized to achieve the largest possible discount and policies 1 and 4 were discarded. Further work may include multi-objective optimization.

4.6 ACKNOWLEDGMENTS

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5

TOWARD A CIRCULAR ECONOMY APPROACH FOR INTEGRATED INTENSIVE LIVESTOCK AND CROPPING SYSTEMS

ABSTRACT

The separation between cropping systems and livestock has caused an imbalance in the nutrients, increasing the environmental impact of both industries. In this work, an integrated system comprising intensive livestock and crop management is compared with traditional systems, from the economic and environmental points of view. A model for estimating energy and nutritional requirements of beef cattle, a waste treatment process, a nutrient recovery system, and crop management is integrated into a mathematical optimization framework. This integrated model allows relating the formulation of the feed of the animals with the composition of their feces, the necessary cultivation area, the crops, and the fertilizers required as well as carrying out the economic and environmental evaluation of the entire system, balancing the nutrients between both industries. Through the application of the model to a representative case study with 1000 animals, a 62% reduction in the environmental impact of the combined agricultural system has been achieved, with a 14% decrease in the profit compared to the non integrated system. The fertilizer formulation is optimized to add exactly the required amount of each nutrient to reduce nutrient pollution. 30% of the nitrogen and 56% of the potassium needed for the crops can be obtained from the livestock waste. The correct formulation of the feed can reduce the amount of phosphorus in the feces down to 0.01%. The results show that the integrated system makes it possible to significantly reduce the environmental impact, but it is still not economically promising yet.

Keywords: product design, circular economy, sustainable processes, integrated crop and livestock systems, beef cattle nutrient recovery, multi-objective optimization

RESUMEN

La separación entre los sistemas de cultivo y la ganadería ha causado un desequilibrio en los nutrientes, aumentando el impacto ambiental de ambas industrias. En este trabajo, se compara un sistema integrado que combina la gestión intensiva de ganado y cultivos tradicionales, desde los puntos de vista económico y ambiental. Un modelo para estimar los requisitos energéticos y nutricionales del ganado bovino, un proceso de tratamiento de residuos, un sistema de recuperación de nutrientes y la gestión de cultivos se integran en un marco de optimización matemática. Este modelo integrado permite relacionar la formulación del alimento de los animales con la composición de sus excrementos, el área de cultivo necesaria, los cultivos y los fertilizantes requeridos, así como realizar la evaluación económica y ambiental de todo el sistema, equilibrando los nutrientes entre ambas industrias. A través de la aplicación del modelo a un estudio de caso representativo con 1000 animales, se ha logrado una reducción del 62% en el impacto ambiental del sistema agrícola combinado, con una disminución del 14% en la ganancia en comparación con el sistema no integrado. La formulación de los fertilizantes se optimiza para agregar exactamente la cantidad requerida de cada nutriente y reducir la contaminación de nutrientes. El 30% del nitrógeno y el 56% del potasio necesarios para los cultivos se pueden obtener a partir de los residuos del ganado. La correcta formulación del alimento puede reducir la cantidad de fósforo en los excrementos hasta el 0.01%. Los resultados muestran que el sistema integrado permite reducir significativamente el impacto ambiental, pero todavía no es económicamente prometedor.

Palabras clave: diseño del producto, economía circular, procesos sostenibles, sistemas integrados de cultivos y ganadería, recuperación de nutrientes en ganado de carne, optimización multiobjetivo.

5.1 INTRODUCTION

Nowadays, the specialization in the production of crops and the intensification of livestock farming has separated both sectors so that dairy or meat production is concentrated in one place and crops are grown in another (Peyraud et al., 2014). This leads to a dependence on mineral fertilizers in crop-growing areas and an excess concentration of nutrients in livestock production areas (Kersberguen, 2020). On the one hand, livestock is one of the main generators of anthropogenic CO_2 (IPCC, 2014). The mismanagement of the waste generated can produce a series of environmental impacts, such as contamination of soils, eutrophication of nearby water resources, or generation of bad odors (FAO, 2006). In addition to these impacts, the emissions from the transportation of animal food to livestock facilities must also be considered. On the other hand, the increase in the population worldwide has pushed crop systems to increase their production and cultivation areas, increasing the consumption of mineral fertilizers. Supplying a higher amount of fertilizers than required by the crops does result not only in an increase in the carbon footprint due to the energy used to obtain the mineral fertilizer but also in problems associated with nutrient pollution such as eutrophication and hypoxia of water bodies (Lammel, 2010).

Some technologies such as anaerobic digestion (Kafle & Chen, 2016), struvite production (Martín-Hernández et al., 2020), and ammonia stripping (Lei et al., 2007) have been used to produce biogas and digestate as a means to reduce the environmental impact of livestock. Nevertheless, most of these studies start directly from a generated waste and analyze whether it is possible to obtain valuable products from it, yet its composition is invariant (Taifouris & Martín, 2018). In addition, it is necessary that the digestate meets certain requirements so that it can be used as a fertilizer (Seadi, 2008).

Integrated crops and livestock systems promote nutrient recycle by converting cellulosic ruminant feed into protein and nutrients from livestock manure into the cell structure of crops (Oltjen & Beckett, 1996). The application of manure through grazing in organic farming has already shown to improve nutrient recycling and pest suppression by promoting soil quality and biodiversity (Carpenter-Boggs et al., 2000; Pimentel et al., 2005; Birkhofer et al., 2008). Whole farm models and nutrient balance approaches, which require the assessment of nutrient reserves, inputs, exports, and losses, can be used to evaluate and establish the best management systems for ruminant production (Dou et al., 1996; Rotz et al., 2007), reducing the environmental impact of agriculture (Badgley et al., 2007). However, even a small imbalance in nutrients can lead to soil depletion or over fertility

(Franzluebbers, 2007). So far, these integrated systems have been developed for small organic farms (extensive livestock) where such integration consists of a grazing activity where manure is deposited naturally (Reddy, 2016) and, to the best of our knowledge, the literature has not analyzed such integration in the case of intensive livestock farming. Models from the literature allow estimating the formulation of the feed based on the age, weight, breed, and sex of the animals, as well as the maintenance costs associated with a livestock farm. Nevertheless, they do not provide the analysis of waste treatment, estimation of the necessary cultivation area, environmental impact, or multi-objective options. To consider these systems, it is necessary to integrate these models into a larger framework.

In this work, an integrated model is developed for the optimal operation of intensive livestock and crop production. The framework integrates a model for estimating energy and nutritional requirements applied to beef cattle, a model of the waste treatment process, and a nutrient recovery system. In addition, the optimization framework considers the area for the crops and other supplementary materials such as water, food supplements, and chemicals. The optimal fertilizer formulation is also considered. A multi-objective (economic and environmental evaluation) approach of the integrated system is carried out, comparing the results with the traditional intensive livestock.

5.2 FRAMEWORK DEVELOPMENT

This work addresses the multi-objective evaluation of an intensive livestock system integrated. First, a model to estimate the energy (energy contained in the food necessary for the maintenance and growth of animals) and nutritional requirements (amount of minerals and proteins) for beef cattle is adapted from the literature (Council, 2000). This model is also used to relate the formulation of the animal feed with the composition of the waste generated. Next, a waste treatment system based on anaerobic digestion is modeled using first principles, such as mass and energy balances, phase equilibrium, and empirical yields. Finally, a nutrient recovery system (ammonia stripping) is included in the framework, modeled using experimental data. Experimental yields are used to estimate the necessary crop area and raw materials to obtain feed for livestock. A fraction of these crops, which is not used for animal feed but is obtained as byproducts, is sold. The environmental evaluation is performed using a composite index, which accounts for the emissions associated with the mineral fertilizers used as well as the water used for irrigated crops. In addition, the integrated system is compared with a nonintegrated one. The following subsections present the different models.

5.2.1 *Model of Energy and Nutritional Requirements for Beef Cattle*

The model developed to determine the energy and nutritional requirements for the cattle in this work is adapted from the model presented in the literature (Council, 2000). The detailed model is shown in the supplementary material. Correlations based on experimental data are used to estimate energy, protein, and mineral requirements throughout the life cycle of the beef cattle, as well as the dry matter intake (DMI) per time unit. Degradation and passage rates are used to analyze the digestion of the feed by the cattle in order to estimate the composition of waste produced. In addition, the energy and nutritional properties and degradation rates of the ingredients considered in this work can be found in the same reference (Council, 2000). Mass and energy balances, together with this information, are used to choose the formulation of the feed and estimate the composition of waste per unit of time.

The time step of the original model is a day. However, to adapt the model to the residence time of the digester, the time unit (TU) is taken to be 24 days (Taifouris & Martín, 2018). The model is reformulated as an optimization problem and extended to include waste treatment and crop management. The growing stages of the beef cattle from birth to slaughter, when the animal is 72-time units old in the case of the cows and 20-time units old in the case of the male yearling, can be seen in Figure 5.1.

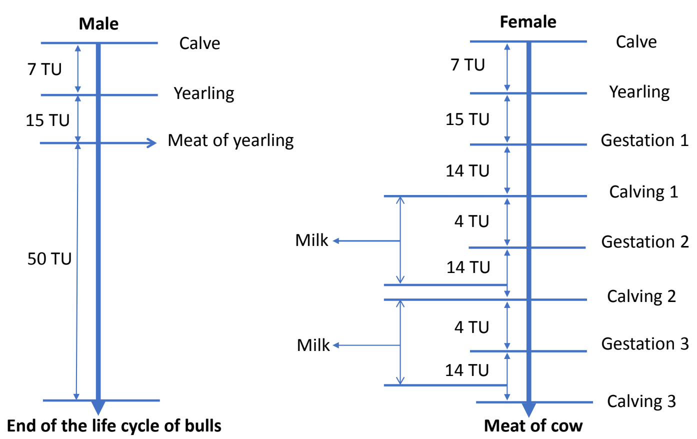

Figure 5.1: Life cycle of the beef cattle by sex.

The growth of cows and bulls is modeled as two uncoupled optimization problems since there are no variables that link both problems. The results are presented together by adding both solutions. In this way, the optimization can be done in parallel. The only data that relates to both models is the ratio of the number of bulls per cow. This value is established before the optimization based on literature information, 1 bull for every 25 cows (Oliveira et al., 2011). The meat of the bulls is not sold. In addition, a series of assumptions are considered:

1. The maximum difference allowed between the energy available and that needed for livestock growth is 10%.

2. Calcium and phosphorus supplements are used for the stages that require it.

The model considers up to 12 different ingredients, which can be consulted in the Supplementary material with their nutritional and energetic properties (Table C.4). It is considered that the surplus of barley grain and wheat straw produced can be sold as a by product if they are not chosen as animal feed. However, the rest of the crops are adjusted to the needs of the animal (whether they are selected as ingredients) so that there are no surpluses for sale. Since the main objective of the exploitation is the production of meat, the crops are sold as byproducts (Lonja de León, 2020). The straw of the rest of the crops is not considered for sale after analyzing the market (Oliveira et al., 2011).

5.2.2 *Waste Treatment*

Anaerobic digestion is used to transform waste into biogas and digestate. The composition of these products depends on the lipids, proteins, and carbohydrates of the waste and can be estimated using a model from previous work (Taifouris & Martín, 2018). The global reactions that are carried out in the digester are as follows:

Lipids:

$$C_{57}H_{104}O_6 + 23.64\,H_2O + 1.45NH_3 \rightarrow 36.36CH_4 + 13.34\,CO_2 + 1.45\,C_5H_7NO_2$$

Protein:

$$CH_{2.03}\,O_{0.6}N_{0.3}S_{0.001} + 0.31\,H_2O \rightarrow 0.41\,CH_4 + 0.42\,CO_2 + 0.030C_5H_7NO_2 + 0.001H_2S + 0.26NH_3$$

Carbohydrates:

$$C_6H_{10}O_5+0.35\,H_2O+0.22\,NH_3 \rightarrow 2.46\,CH_4+2.46CO_2+0.22C_5H_7NO_2$$

This model uses these stoichiometric ratios and experimental conversions to estimate the composition of the products and water and ammonium requirements. These and other considerations can be found in the supplementary material.

Biogas upgrading is performed using a bed of Fe_2O_3 to remove H_2S, a scrubber to reduce the ammonia content down to 5%, and a pressure swing adsorption system to remove water, CO_2, and ammonia (León & Martín, 2016). The stoichiometric ratios and adsorption yields, found in the Supporting Information, are used to estimate the final biogas composition and size of the adsorbent bed required.

5.2.3 *Nutrient Recovery Systems.*

The liquid and solid effluents, which exit the digester, are separated using a decanter centrifuge. It is considered that 25% of the ammonia is retained by the solid phase (Holm-Nielsen et al., 2009) and is lost in the storage process, while the liquid effluent is treated by an ammonia-stripping process, which can recover 89% of the ammonia dissolved (Lei et al., 2007). It is necessary to use 27.5 g $Ca(OH)_2$ per liter of effluent to promote the formation of ammonia and 2.88 kg of H_2SO_4 per kilogram of NH_3 recovered (Lei et al., 2007).

The liquid effluents from the different stages of the ammonia stripping process are stored together with the solid effluent from the decanter and are naturally dried in a controlled warehouse, ensuring that the phosphorus and potassium amounts are maintained in the final product. The amount of phosphorus and potassium recovered is the difference between the one required for the animals and that supplied with the feed and supplements. The mass balances as well as the process flowsheet can be found in the Supporting Information.

5.2.4 *Crops Growing and Management.*

The work considers the most common crops that can be used for animal feed. On the one hand, the relationship between the amount of each crop and the required crop area is estimated using yields from the literature (Bellido, 2010; Ministerio de Agricultura, pesca y alimentacion, 2019). On the other hand, technical reports are used to obtain the water (InfoRiego, 2014) and fertilizer (Bellido, 2010) requirements and the cost of crop production (tillage, sowing, and harvesting) (Ministerio de Agricultura pesca y alimentación, 2019). The reference considers fertilizer losses due to leaching and an average concentration of nutrients present in the soil to estimate the amount of fertilizer per unit of hectare, and therefore, it is not necessary to add a correction factor.

This information as well as the completed list of the crops can be found in Table C.3 in the supplementary material. Storage is necessary to ensure the availability of all types of crops throughout the year since there are crops that grow in spring and others that grow in winter.

5.2.5 *Fertilizer Formulation.*

Fertilizer formulation is calculated to avoid any excess or deficiency of nutrients in the soil. Ammonium nitrate (34-0-0), simple superphosphate (0-20-0), and potassium sulfate (0-0-50) (Agrifeed, 2021) are used to supply nitrogen (0.34 kgN/kg), phosphorus (0.20 kgP2O5/kg), and potassium (0.50 kgK2O/kg) to the soil, respectively. The amount of each type of fertilizer is fixed by using mass balances, which can be found in the supplementary material, between the nutrients recovered from the digestate and the nutrients required from the selected crops.

5.2.6 *Environmental Impact Index.*

Global warming potential (GWP), eutrophication potential (EUp), and water footprint (WF) are used to analyze the impact of the integrated livestock system. Technical reports (Skowroñska & Filipek, 2014) are used to obtain the values of GWP and EUp per ton of fertilizer, while the water footprint is estimated as the water consumed by irrigation (see Section 5.2.4).

A composite index is developed to consider simultaneously the different impacts. The indexes (I_i) are standardized (In_i) using the minimum-maximum standardization approach (Eq.(5.1)), and an additive aggregation method (Eq. (5.2)) (Nardo et al., 2008) is used to compute the composite indicator (CI). The weights are estimated using a technical report (Serenella et al., 2018).

$$\mathrm{In_i}= \frac{\mathrm{I_i\text{-}min\ (I_i)}}{\mathrm{max\ (I_i)\text{-}min\ (I_i)}} \qquad \mathrm{i} \in [GW, EUp, WF] \tag{5.1}$$

$$\mathrm{CI}= \sum_i \mathrm{weight}_i \cdot \mathrm{In_i} \tag{5.2}$$

The values of GWP, EUp, and WF per ton of each type of fertilizer as well as the weights of each index are found in Table C.1 in the Supporting Information.

5.2.7 *Solution Procedure*

The objective function is based on the profit (Pro), and it is shown in Eq.(5.3).

$$\begin{aligned}&\text{Pro=In}_{\text{M}}\text{+In}_{\text{P}}\text{+In}_{\text{crops}}\text{+In}_{\text{bio}}\text{-Cst}_{\text{growth}}\text{-Cst}_{\text{Field}}\\&\text{-Cst}_{\text{Fertilizer}}\text{-Cst}_{\text{Storage}}\text{-Cst}_{\text{Suplement}}\text{-Cst}_{\text{Manpower}}\text{-Cst}_{\text{Aux}}\end{aligned} \tag{5.3}$$

The terms In_{M}, In_{P}, In_{crops}, and In_{bio} correspond to the income of meat, potential, crops, and biogas, respectively. The income from the meat (In_{M}) is calculated by Eq.(5.4).

$$\text{In}_{\text{M}}\text{= In}_{\text{Cows}}\text{+In}_{\text{YearlingM}}\text{+In}_{\text{YearlingF}} \tag{5.4}$$

Where In_{Cows}, $\text{In}_{YearlingM}$, and $\text{In}_{YearlingF}$ are the incomes from the sale of cows, male yearling, and female yearling, respectively. Each income can be estimated using their final weights, the meat yield, and the official price of the meat from the literature. The potential income (In_{P}) is the profit that can be obtained out of the new calves, which are gestated along the life cycle of cows (see Figure 5.1) when they become yearling and are sold. During its life cycle, each cow can give birth up to three calves. This income is calculated by Eq.(5.5).

$$\text{In}_{\text{P}}\text{= NA}_{\text{CalNew}} \cdot \text{Pot} \tag{5.5}$$

Where NA_{CalNew} corresponds to the new calves that can be male or female. Pot is the potential value of the calves and is calculated as the difference between the selling price of the yearling and the feeding costs of calves and yearlings.

The income obtained from the crops (In_{crops}) is calculated by Eq.(5.6).

$$\begin{aligned}&\text{In}_{\text{Crops}} = \text{BarlGn} \cdot \text{Pri}_{\text{Barley}} + \text{BarlSw} \cdot \text{Pri}_{\text{Barley.Straw}} +\\&\text{WhtGn} \cdot \text{Pri}_{Wheat} + \text{WhtSw} \cdot \text{Pri}_{Wheat.Straw}\end{aligned} \tag{5.6}$$

BarlGn and BarlSw correspond to the amount of barley (grain and straw, respectively) that is not used as animal feed and can be sold. WhtGn and

WhtSw represent the rest of the wheat plant (grain and straw) that can also be sold. Both crops can be used as animal feed, and therefore the model selects the destination of these crops based on the objective function. The prices, Pri_i, are reported in Table C.3 in the Supporting Information. The income obtained from selling biogas (In_{bio}) is calculated by Eq. (5.7).

$$\mathrm{In_{bio}}{=}\mathrm{Amt}_{biogas} \cdot \mathrm{yd}_{Biogas} \cdot \mathrm{Pri_{power}} \tag{5.7}$$

Where Amt_{Biogas} is the amount of purified biogas. The yield to the power is assumed to be 40%, and the heat of combustion takes the value of 14 kWh (Instituto para la diversificación y ahorro de energía (IDAE), 2020) per kilogram of biogas (yd_{Biogas}). Pri_{power} is the sale price of power produced using biogas from livestock manure and its value is 200 €/MWh (Llorens, 2018). The crop production cost of each ingredient (Cst_j) is the sum of the cost of tillage, sowing, and harvesting (Eq. (5.8)) (this cost does not include the cost of fertilizer, field, manpower, and storage) and can be found in Table C.3 in the Supporting Information.

$$\mathrm{Cst_j} = \mathrm{Cst_{Tillage_j}}{+}\mathrm{Cst_{Sowing_j}}{+}\mathrm{Cst_{harvesting_j}} \tag{5.8}$$

Cst_{growth} is the cost of production of the crop fed to calves (Cst_{Calves}), yearlings ($Cst_{Yearling}$), cows (Cst_{Cow}), and bulls (Cst_{bulls})(Eq.5.9).

$$\mathrm{Cst_{growth}} = \mathrm{Cst_{Calves}}{+}\mathrm{Cst_{Yearling}}{+}\mathrm{Cst_{Cow}}{+}\mathrm{Cst_{Bull}} \tag{5.9}$$

These costs are calculated using the DMI per TU (DMIt), the number of each type of animal (NA_{calves}, $NA_{yearling}$,NA_{cows}, and NA_{Bulls}), and the crop production cost of the feed (Cst_{Mt}), which depends on the Cst_j and the proportion of each ingredient 'j' in the feed($x_{t,j}$). All-female calves are grown into cows, while male calves are grown into meat. Between TU 0 and TU 6, the animals are calves, between 7 and 20 are yearlings, and between 21 and 72 can be cows or bulls. The crops profit (Pro_{crops}) is defined by Eq.(5.10)

$$\mathrm{Pro}_{crops} = \mathrm{In}_{Crops} - \mathrm{Cst_{growth}} \tag{5.10}$$

The rest of the costs are calculated by Eqs.(5.11)-(5.15). These costs correspond to renting the field needed to grow the crops (Cst_{Field}), the mineral fertilizers ($Cst_{Fertilizer}$), the storage cost of the crops ($Cst_{Storage}$), the cost of labor ($Cst_{Manpower}$), and the auxiliary cost (Cst_{aux}). These costs are not included in Cst_{growth} to facilitate the analysis of results.

$$\mathrm{Cst_{Field}}{=} \mathrm{Pri_{Rent}} \cdot \mathrm{AreaT} \cdot \mathrm{LC_{animal}} \tag{5.11}$$

$$\mathrm{Cst}_{\mathrm{Fertilizer}} = \mathrm{Amt}_{\mathrm{N}} \cdot \mathrm{Pri}_{\mathrm{N}} + \mathrm{Amt}_{\mathrm{P}} \cdot \mathrm{Pri}_{\mathrm{P}} + \mathrm{Amt}_{\mathrm{K}} \cdot \mathrm{Pri}_{\mathrm{K}} \tag{5.12}$$

$$\mathrm{Cst}_{\mathrm{Storage}} = \mathrm{Pri}_{\mathrm{storage}} \cdot \left(\sum_{t} \mathrm{DMI}_{t}\right) \cdot \frac{\mathrm{LC}_{\mathrm{animals}}}{\mathrm{LC}_{\mathrm{silo}}} \tag{5.13}$$

$$\mathrm{Cst}_{\mathrm{ManPower}} = \mathrm{Pri}_{\mathrm{MP}} \cdot \mathrm{AreaT} \tag{5.14}$$

$$\mathrm{Cst}_{\mathrm{Aux}} = \mathrm{Cst}_{\mathrm{WaterAgri}} + \mathrm{Cst}_{\mathrm{WaterLiv}} + \mathrm{Cst}_{\mathrm{water}} + \mathrm{Cst}_{\mathrm{Supl}} + \mathrm{Cst}_{\mathrm{Bass}} + \mathrm{Cst}_{\mathrm{Acid}} \tag{5.15}$$

The field used to grow the crops is rented at a price of 137€/ha·yr (Junta de Castilla y León, 2019) (Pri_{Rent}), while AreaT is the maximum total area used per year. The prices of ammonium nitrate (Pri_{N}), superphosphate (Prin_{P}), and potassium sulfate (Prin_{K}) are 334, 202, and 353 €/t (Ministerio de Agricultura Pesca y Alimentación, 2020), respectively. The price of storing the crops (Pristorage)is 26 €/t (Biroccesi, 2000). LC_{silo} is the life cycle of the silo (25 years), while $\mathrm{LC}_{animals}$ is the life cycle of the animals (6 years, see Figure 5.1). The cost of labor is calculated using the price of manpower per unit of area (Pri_{MP}), whose value is 50 €/ha (Ministerio de Agricultura Pesca y Alimentación, 2017). The auxiliary costs (Cst_{Aux}) correspond to the cost of water in the case of the irrigate crops ($\mathrm{Cst}_{WaterAgri}$) (corn is the only irrigate crop considered in this work), water for the beef cattle ($\mathrm{Cst}_{WaterLiv}$), nutritional supplement of calcium and phosphorus (Cst_{Supl}), calcium hydroxide (Cst_{Bass}), and sulfuric acid (Cst_{Acid}) necessary to recover nitrogen. Further details are included in the supplementary material. In addition, a new constraint must be added in the optimization framework to limit the use of the supplement of phosphorus (Eq.(5.16)).

$$\mathrm{Amt}_{\mathrm{Supl}_{t}} \leq \mathrm{Pneed}_{t} \tag{5.16}$$

Where Amt_{Supl_t} is the amount of supplement of phosphorus in the TU "t" and Pneedt is the phosphorus requirement of the beef cattle in the TU "t".

In the multiobjective case, the ε-constraint method is used to include the environmental objective (composite index) into the solution procedure.

5.3 RESULTS AND DISCUSSION

One thousand calves are used as a starting point (500 females and 500 males). The female calves grow into cows, producing three new animals (which can be two males and one female and vice versa). Two results are presented, the optimal economic and the multi-objective, considering both the economic and the environmental objectives. It is considered that the soil has an average concentration of nutrients.

5.3.1 *Optimal Economic Solution*

After carrying out an analysis of the feed formulations in each of the time units during the life cycle of the animals, it is observed that the main changes occur in time units 21 and 37, corresponding to the first and second gestations. Therefore, the average formulations between the time units 0-20 (first stage), 21-37 (second stage), and 38-72 (third stage) can be used, which can be seen in Figure 5.2.

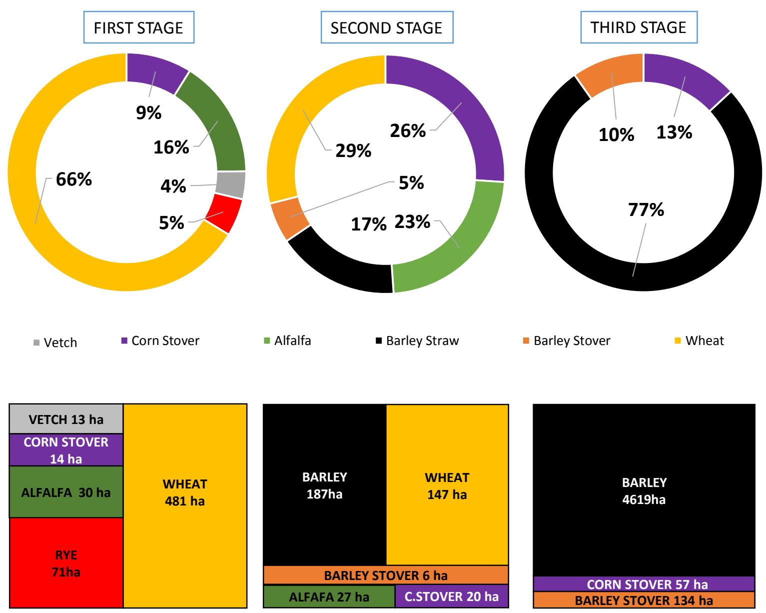

Figure 5.2: Optimal formulation of the feed and cultivation areas in the economic scenario.

During the first stage, the main ingredients are wheat, alfalfa, and corn stover. For the first stages of growth of the animals, the amount of feed ingested is small and the energy needed for growth and maintenance is high; therefore, it is necessary to use high-density energetic crops (concentrate intakes). Among the most energetic concentrates are corn and wheat grain (see Table C.4) in the Supporting Information). Corn has a lower crop production cost than wheat (0.02 vs 0.04 €/kg), but as it is an irrigated crop, water consumption must also be considered. Therefore, with the cost of water, the production cost of corn reaches 0.11 €/kg, which is higher than that of wheat. As a result, the consumption of wheat is prioritized. Rye is also used as an energy crop. The consumption of alfalfa, corn stover, and vetch provides the largest fraction of the minerals required. Nevertheless, calcium and phosphorus supplements are necessary to meet the nutritional requirement (63 t), which represent 0.64% of the total feed of all animals.

When the animals are older, along the second stage, the DMI is higher and the energy required per mass of feed is lower; therefore, the feed formulation tends to use less concentrates. In addition, during this second stage, the cows are gestating and begin to produce milk, requiring a larger amount of minerals and proteins. The feed formulation changes toward a higher concentration of forage compared to the previous stages (71% vs 29%) since forage has a higher concentration of minerals than the concentrated ingredients. In addition, changes are observed in the type of forage. Vetch is replaced by barley straw. This is because a lower amount of energy is required in this section, which can be supplied by straw. In the third stage, a gradual increase in the presence of forage, mainly barley straw, is observed in the formulation of the feed, reaching values of 100%. The use of barley straw involves the production of barley grains since both come out of the barley crop. The barley grains can be sold, obtaining an additional income. For this reason, it is the main crop produced.

The area required for the cultivation of each of the crops can also be seen in Figure 5.2. In the first stage, most of the cultivated area is devoted to wheat, with a small area used for the cultivation of rye, alfalfa, corn stover, and vetch. From the second stage, the cultivation of rye, vetch, and wheat are displaced by the cultivation of barley due to the less need for concentrates (since only barley straw is used for animal feed) and the large benefit that the sale of barley grain provides. This trend is consolidated in stage 3 where the main crop is barley. Furthermore, if the necessary cultivation area is analyzed year by year, it can be concluded that the last years require a much larger area than the first ones since the animals need less food when they are younger. Since the maximum area needed is rented from the first year, but it is not used for animal feed, it can be used to obtain an additional profit by selecting a crop that does not cause a strong deterioration of the soil. However, this possibility has not been considered in this work, to focus the study on livestock.

A sensitivity study is carried out by changing the objective function to minimize and maximize the nitrogen, potassium, and phosphorus needed (N_{nd},K_{nd}, and P_{nd}) and nitrogen, potassium, and phosphorus recovered (N_{rec},K_{rec}, and P_{rec}), respectively, instead of the profit (see Eq.(C.129)-(C.131) and Table C.3) in the Supporting Information). In addition, the results of the economic scenario are also included in this study as "optimal". The results are shown in Table 5.1.

Table 5.1: Nutrient's balance and requirement of fertilizer in the economic scenario

Scenario		Needed(t)			Recovered(t)			Fertilizer needed(t)
Objective Function	Type	N	P	K	N	P	K	
MinN	Needed	212	149	483	121	25	284	1291
MinP		231	102	461	88	24	297	1129
MinK		240	105	459	87	24	291	1185
MaxN		599	258	655	111	25	266	3397
MaxP		562	261	623	115	27	269	3227
MaxK		428	187	715	101	30	229	2666
MinN	Recovered	293	127	509	84	26	284	1566
MinP		303	177	583	114	0.3	252	2098
MinK		347	154	589	97	30	204	2055
MaxN		216	177	518	139	25	277	1481
MaxK		405	176	478	102	22	305	2052
MaxP		333	183	569	126	42	260	1920
Optimal		328	159	584	95	0.4	264	2109

It is observed that the amount of phosphorus recovered is extremely low in the "optimal" case. This is because the model prioritizes the reduction of fertilizer consumption by using crops that consume fewer nutrients. In the case of phosphorus, the most used ingredient, barley straw, is one of the crops with the lowest phosphorus content (see Table C.4 in the Supporting Information), so its content in the feces is low. For this reason, it is necessary to use phosphorus supplements to compensate for this deficiency in some stages.

A correct selection of ingredients in the feed and, therefore, of the crops, can reduce the amount of additional N, P, and K down to 2.85, 2.55, and 1.55 times, respectively. The margin of difference between the maximum and minimum values of N and K recovered is much smaller. In this case, it is possible to increase the amount of N 1.65 times and 1.49 times in the case of K. In the case of phosphorus, the amount varies between almost total adjustment with the requirements of the animal, as it occurs in the optimal case, up to almost 40 tons recovered. This indicates that the correct selection of crops, together with rational use of feed supplements, could substantially reduce the amount of this nutrient in livestock waste.

On the one hand, the crops selected in the economic scenario show a consumption in the middle of the maximum and the minimum value in the three nutrients. This is so because there is a balance between the crop production cost, the fertilization costs, and the sales income. On the other hand, in the case of nutrients recovered, there are clear differences. Nitrogen is close to the minimum since the selected crops do not allow a higher recovery and priority is given to reducing the necessary nitrogen versus increasing the nitrogen recovery, to reduce the difference between the two and thus the contribution of nitrogen fertilizer. Despite this, the nitrogen recovered represents 29% of the total required. Finally, the amount of potassium recovered is situated between the maximum and minimum possible values, representing 45% of the necessary value.

5.3.2 *Multiobjective Feed Design*

First, the upper and lower limits of the three different indexes are calculated to compute the composite index, CI. These values are shown in Table C.2 in the Supporting Information. The relationship between the composite index and the maximum profit obtained during the complete cycle of the animal can be seen in Figure 5.3.

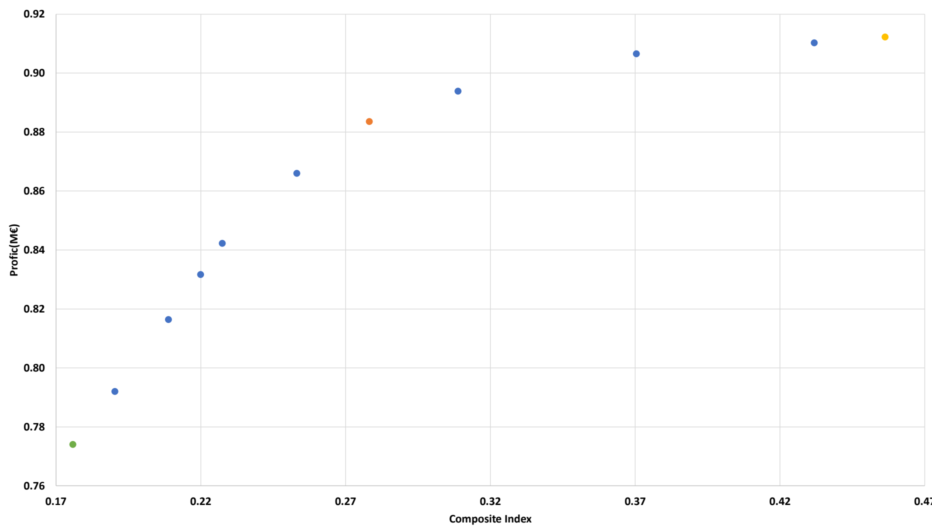

Figure 5.3: Pareto curve for the design of the feed formulation (green:ecofriendly scenario, orange: multi-objective scenario, and yellow:economic scenario).

There are two regions clearly delimited by a point from which profits begin to fall sharply, 0.28. Therefore, three scenarios can be considered, the economic (CI = 0.46), the multiobjective (CI = 0.28), and the eco-friendly (CI = 0.18).

A techno-economic evaluation is carried out to understand the change in the slope, and the main results are presented in Figure 5.4.

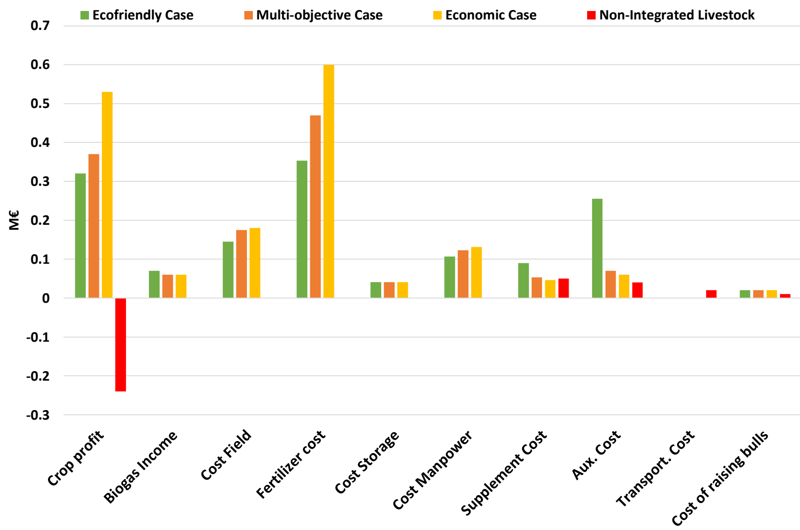

Figure 5.4: Techno-economic analysis of the different considered scenarios.

The case of the nonintegrated system is also included in the comparison. The incomes or costs that have the same value for all the scenarios considered are not included in the Figure, but they can be found in Table C.6 in the Supporting Information, together with a more detailed information of this evaluation.

Between the economic scenario and the multiobjective one, a slight decrease in profit down to 3% is observed, but a large decrease in the composite environmental index of 39% is achieved, which turns this point into a tradeoff between the cases of economic and environmental optima. The decrease in the profit is limited because the loss in the profit from the crops (the difference between the income for the sale of the crops and the costs of their cultivation, (see Eq.(5.10)) is partially offset by the savings in fertilizer costs, the renting cost of the field, and the manpower cost due to the changes in the crops and the area used. There are three reasons for the drop in income from the sale of crops: the reduction of the cultivation of barley, the use of a part of the barley grains for animal feed, and the reduction of the cultivation of wheat, whose straw is also sold. In addition, the change of crops from corn stover (0.019 €/kg) to barley stover (0.058 €/kg) increases the crops' production cost.

A faster decrease in profit is observed with respect to the composite index between the multiobjective and eco-friendly scenarios. In this region, 36% of the total variation in CI corresponds to 80% of the total variation in profit.

This occurs due to two important changes in the formulation of the feed. Wheat and rye are replaced by corn, which requires an artificial water supply, increasing the auxiliary costs. In addition, there is a significant decrease in income from crop sales due to lower barley production (13524 t vs 15124 t) and wheat substitution. These changes reduce fertilizer consumption (1323 t vs 1651 t) and, therefore, the fertilizer cost. Nevertheless, the savings in fertilizer cost does not compensate for the increase in the auxiliary costs and the decrease in the income from the crops. Therefore, the drop in the profit is so prominent between these scenarios.

The nonintegrated case can be seen as an extreme case of the economic scenario of the integrated system since it has a higher benefit (1.03 M€) than any of the integrated scenarios (11.67% higher than the economic case and 14.5% higher than the multi-objective case) but also a larger environmental impact, with a composite index of 0.74, 76% higher than the eco-friendly case.

A difference can be observed between the profit of the crops in the integrated and nonintegrated cases. The main reason is that to produce straw in the integrated cases, it is necessary to cultivate the cereal and include the crop production cost. Later, the straw is used for animal feed while the grain can be sold, obtaining an income that compensates for the crop production cost. In fact, in the three integrated cases, the income from selling the crops outweighs the crop production costs, resulting in a profit. Given that the nonintegrated case does not require the cultivation of cereal to obtain the straw, because it is bought directly from a distributor, acquisition costs are lower (0.035 €/t), despite these costs including the costs of fertilizer, storage, labor, and land. For this reason, these costs are equal to 0 for the nonintegrated case, as can be seen in Figure 5.4. However, the income from the crops is also zero, and therefore, the crop profit is negative. However, the total cost of the integrated scenarios is higher than the costs of the nonintegrated scenario due to the rest of the costs, which do not include the crop production cost (field, fertilizer, storage, manpower, supplement, and auxiliary), making the non-integrated case the most profitable from an economic point of view. This result is in line with the current situation of both industries, which tends toward a specialization of crops to seek the highest economic performance through economies of scale. However, the environmental impact of the nonintegrated scenario is the highest of all the cases presented, with fertilizer consumptions 19% higher with respect to the economic scenario, 36% higher than the multiobjective scenario, and 49% with the eco-friendly scenario. In addition, the GWP per consumer benefit (CB), that is, 1 kg of consumed, boneless, edible beef in the United States, is calculated corresponding to 29% of the live weight (Asem-Hiablie et al., 2019). The total weight of the yearlings and cows slaughtered is 440 t, and therefore, the CB is 127.6 t. The values of GWP for the cases considered in this work can be found in Table C.6 in the Supporting Information. The values obtained are 5.27, 7.87, 10.1, and 13.73 $kgCO_2$ eq per CB for the eco-friendly, multi-objective, economic, and nonintegrated cases, respectively. These values are comparable with others found in the literature such as 8 and 10 $kgCO_2$ eq/CB (Asem-Hiablie et al., 2019).

In the case of the breeding of bulls, only the economic impact has been considered because the environmental impact is not significant compared to that of cows (2% in the footprint and 1.7% in the eutrophication potential), and therefore, there is no additional interest in finding a tradeoff between the economic and environmental optimum. For this reason, the cost is the same in all three scenarios.

For the multiobjective case, the optimal formulations for each stage can be found in Figure 5.5. It is observed that the main changes occur at the same points as in the case of the economic optimum, so the same procedure described in the previous section is used here.

In the first months of the life of the animals, the results of the multi-objective scenario are slightly different from the economic optimum. On the one hand, alfalfa, and corn stover are completely replaced by barley stover since this crop has a lower requirement of phosphorus and potassium.

Similar to the optimal economic case, during the second growth phase, an increase in the amount of forage consumed is observed (70% vs 28%), which is supplied by a mixture of corn stover, barley straw, and barley stover. The most important change is the use of barley grain as an energy crop (concentrate) instead of wheat, saving area and fertilizer. This causes a reduction in the income because this part of the barley crop was destined for sale in the economic case, and in this case, at least a fraction of it is used for animal feed.

In the last stage, the energy needs are even lower and the nutritional and mineral needs are higher. Therefore, the amount of forage is higher (100%) and the barley grain and wheat are totally replaced by barley straw and barley stover. The fraction of barley straw is lower than in the economic case, and therefore, the sales income is also lower.

In Figure 5.5, the areas needed for each crop for the three stages can also be observed. The discussion is similar to the analysis of the crop

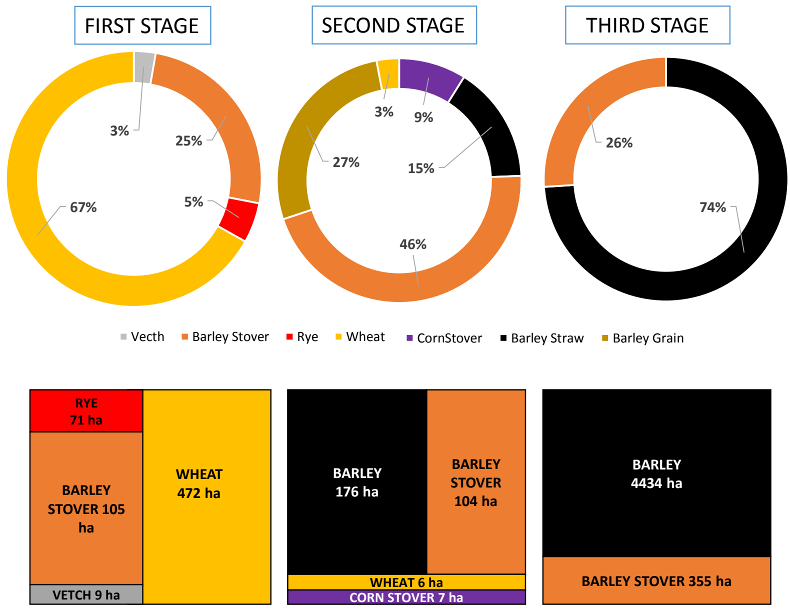

Figure 5.5: Optimal formulation of the feed and cultivation areas in the multi-objective scenario.

portfolio. The total area and the fertilizer consumption are lower than in the economic case and, therefore, the environmental impact is also lower.

A sensitivity study is also performed for this case. Unlike the values presented in Table 5.1 (economical optimum), it can be observed that the optimal values for the fertilizers tend more toward the minimum with a value of 284 tons of nitrogen, 125 tons of phosphorus, and 513 tons of potassium since the environmental impact has been limited compared to the economic case and a part of the economic benefit must be sacrificed to reduce the amount of fertilizer needed. In the case of nutrients recovered, 86 tons of nitrogen and 290 tons of potassium are recovered, which represent 30 and 56% of the nitrogen and potassium needed, respectively. These values are consistent with other studies in literature, with values of 23% for nitrogen (Franzluebbers, 2007) and 50% for potassium (Mukhlis et al., 2018).

5.4 CONCLUSIONS

In this work, an integrated model has been developed to optimize self-sufficient intensive livestock systems considering the management of waste and the crops necessary for the nutrition of the animals. Waste treatment and nutrient recovery favor a circular economy. The techno-economic analysis of the farm has been carried out and a composite index has also been developed, including the effect on the atmosphere and the water resources of the fertilizers used, as well as the water consumed, to evaluate the environmental impact.

The results show that it is possible to significantly reduce the environmental impact down to 62% of a livestock farm by assuming a loss of 14% (between the nonintegrated and the multiobjective case) in the profit, that can be compensated for with some incentives oriented to the development of sustainable operation of livestock facilities (Martín-Hernández et al., 2021). Since in the integrated cases, the nutritional and mineral requirements can be covered by a large variety of ingredients, the appropriate selection of crops allows reducing the environmental impact down to 39%, keeping the reduction in the profit within 3% (between the economic and multi-objective cases of the integrated systems), opting for a tradeoff between the economic and environmental objectives. In addition, the model designs a fertilizer that, for the selected crops, balances the amount of nutrients supplied and required, reducing the possibility of overfertilization of the land.

The sensitivity analysis shows that it is possibleto substantially reduce the environmental impact by minimizing the nutrients needed for the crops, as these can be reduced to three times in some cases. Furthermore, by correctly adjusting the phosphorus supplied through feed supplements and crops, it is also possible to substantially reduce its presence in the residues. Finally, note that an important fraction of the nutrients, up to 41%, can be recovered from the animal feces and the crop surpluses have been sold to improve the economic performance of the system.

5.5 ACKNOWLEDGMENTS

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6

INTEGRATING INTENSIVE LIVESTOCK AND CROPPING SYSTEMS: SUSTAINABLE DESIGN AND LOCATION

ABSTRACT

CONTEXT: A mismatch between nutrient demand and consumption in livestock and cropping systems makes these sectors responsible for 24.5% of greenhouse gas emissions. In order to reduce the gap between the two industries, approaches focused on integrating livestock and crop management have been presented. Location is a key factor in the sustainable operation of these integrated systems since this variable affects both the economic and environmental dimensions of the design of the farm.

OBJECTIVE: In this work, a two-step methodology is proposed to address simultaneously the formulation of the feed, the design of the nutrient recovery process, the location of the facilities, and its size, from economic and environmental points of view.

METHODS: First, prescreening is used to discard locations that do not meet a series of environmental constraints. Next, an optimization framework is developed by integrating empirical models that estimate the nutritional needs of the animals, fertilizer consumption, waste production, as well as the effect of selection of locations and the size of the farm on the objective function. The farm is designed to produce the feed on the premises and animal wastes are used to produce fertilizers and biogas, implementing the circular economy. The optimization framework is used to estimate the optimal feed formulation, crop selection, size and location, following a multi-objective approach.

RESULTS AND CONCLUSIONS: The methodology is applied to a case study in Spain. Of the 345 agricultural districts considered, 145 are discarded in the prescreening. The optimal number of initial animals is 1000. The results show that the selection of 'Bureba-Ebro' and a crop distribution that consumes 12% less nutrients than the economic scenario, results in the reduction of 35% in the environmental impact. In addition, meat production cost is 8.87€/kg (1.6€/kg corresponds to the waste treatment). Nevertheless, it can be reduced down to 1.51€/kg by considering the income from crop sales.

SIGNIFICANCE: Only through this integrated framework it is possible to determine the feed formulation and facility location that best balance the economic and environmental objective, and determines the percentage of nutrients that can be recovered. The methodology is generic enough to be applied to other locations, crops, and animals.

Keywords: Crops management, Sustainable design, Livestock Industry, Circular Economy

RESUMEN

CONTEXTO: Un desajuste entre la demanda y el consumo de nutrientes en los sistemas de cultivo y ganadería hace que estos sectores sean responsables del 24,5% de las emisiones de gases de efecto invernadero. Con el fin de reducir la brecha entre las dos industrias, se han presentado enfoques centrados en la integración de la gestión de la ganadería y el cultivo. La ubicación es un factor clave en el funcionamiento sostenible de estos sistemas integrados ya que esta variable afecta tanto a las dimensiones económicas como ambientales del diseño de la granja.

OBJETIVO: En este trabajo, se propone una metodología de dos pasos para abordar simultáneamente la formulación del alimento, el diseño del proceso de recuperación de nutrientes, la ubicación de las instalaciones y su tamaño, desde puntos de vista económicos y ambientales.

MÉTODOS: Primero, se utiliza una preselección para descartar las ubicaciones que no cumplen una serie de restricciones ambientales. A continuación, se desarrolla un marco de optimización mediante la integración de modelos empíricos que estiman las necesidades nutricionales de los animales, el consumo de fertilizantes, la producción de residuos, así como el efecto de la selección de ubicaciones y el tamaño de la granja en la función objetivo. La granja está diseñada para producir el alimento en las instalaciones y los residuos animales se utilizan para producir fertilizantes y biogás, implementando la economía circular. El marco de optimización se utiliza para estimar la formulación óptima del alimento, la selección de cultivos, el tamaño y la ubicación, siguiendo un enfoque multiobjetivo.

RESULTADOS Y CONCLUSIONES: La metodología se aplica a un estudio de caso en España. De los 345 distritos agrícolas considerados, se descartan 145 en la preselección. El número óptimo de animales iniciales es de 1000. Los resultados muestran que la selección de "Bureba-Ebro" y una distribución de cultivos que consume un 12% menos de nutrientes que el escenario económico, resulta en la reducción del 35% en el impacto ambiental. Además, el costo de producción de carne es de 8,87€/kg (1,6€/kg corresponde al tratamiento de residuos). Sin embargo, se puede reducir hasta 1,51€/kg considerando los ingresos por ventas de cultivos.

SIGNIFICADO: Solo a través de este marco integrado es posible determinar la formulación del alimento y la ubicación de las instalaciones que mejor equilibren el objetivo económico y ambiental, y determinar el porcentaje de nutrientes que se pueden recuperar. La metodología es lo suficientemente genérica como para aplicarse a otras ubicaciones, cultivos y animales.

Palabras clave: Gestión de cultivos, Diseño sostenible, Industria ganadera, Economía circular.

6.1 introduction

Livestock and cropping systems represent two of the largest sources of greenhouse gas emissions, accounting for 24.5% of total global emissions (U.S. Environmental Protection Agency, 2021). The decoupling of both sectors has led to a mismatch between sources of nutrients through livestock waste and areas with high requirements of these. This results in nutrient pollution, leading to eutrophication and soil deterioration (Peyraud et al., 2014), as well as a significant carbon footprint due to the extraction, treatment, and transport of mineral fertilizer. Regarding livestock waste, several treatment processes have been proposed, including composting, anaerobic digestion (Loyon, 2017), and nutrient recovery (Martín-Hernández et al., 2021). Nevertheless, the cost associated with these processes, as well as the transportation of the products from livestock areas to crop areas, can be economic and environmental bottlenecks for the sustainable use of these wastes (Case et al., 2017; Makara & Kowalski, 2018).

With the aim of bridging the gap between the two industries, approaches focusing on the integration of livestock and crop management have been presented. These integrated systems have several advantages beyond reducing transportation costs, such as increasing crop yields and nutrient use efficiency, as well as decreasing total greenhouse gas emissions, and maintaining soil quality (Moraes et al., 2014). All these advantages are aimed at promoting the circular economy of waste and achieving zero waste emission. However, most of these studies have focused on extensive livestock farming (Bell et al., 2014; Sulc & Franzluebbers, 2014) when the real problem lies in intensive livestock farming (Tullo et al., 2019). While extensive farming has several advantages over intensive farming (preservation of the natural environment, ecosystem, government support, less environmental impact, and resource consumption), it has an important disadvantage, its productivity. As a result, the food generated by this type of farming is more expensive than intensive farming, requires a higher land use and more labor (Novikova & Startiene, 2018). Therefore, intensive farming is necessary to supply food in an economically sustainable way to a growing population. Authors, such as Taifouris and Martin, 2021 have addressed this type of integration for intensive livestock farming. Through models for estimating energy and nutritional requirements, waste treatment, nutrient recovery, and crop management, it is possible to determine the optimal feed formulation for the animals, the required crops, as well as the operating conditions of the waste treatment process, and the optimal formulation of fertilizers. By establishing a multi-objective approach, these models suggest an optimal solution that is a trade-off between the economic and environmental optimums. However, the proposed design misses the effect of localization of the facility.

Location is a key factor since it determines the growing yield of the crops, through climate and soil characteristics (Liliane & Charles, 2020; Mechiche-Alami & Abdi, 2020). In addition, the location selected also determines the availability and cost of the land and water. These parameters affect both the economic performance and the environmental impact of the farm. The design of the product (feed), the process (waste treatment and nutrient recovery) and the selection of the location are closely related and synergistic. Depending on the location, the crops with the highest production yields in that agricultural district are selected, favoring some feed formulas over others. In the same way, the process design depends on the composition of the residues (Weinrich & Nelles, 2015) and that is a function of the feeding of the animals (Council, 2000). In addition to the parameters related to the economic aspects of the farm, there are environmental constraints (nitrate vulnerable zone, natural parks, and water scarcity) that limit the location of this type of facility. Integrated product and process design and, ultimately, three-dimensional concurrent engineering (3DCE) have proven to be the most efficient way to design production systems (Ellram et al., 2007). However, its application has been rather limited and focused on the chemical industry, (Gani, 2004; Bernardo & Saraiva, 2005; Martin & Martinez, 2013), leaving the food industry with a limited number of studies, (Almeida-Rivera et al., 2007), and even less in the case of animal feed (Csikai, 2011). Therefore, the development of a methodology to systematically select the best feed formulation, crops, process conditions, size, and locations is paramount to globally address the design of livestock-cropping systems. To the best of the knowledge of the authors, the integrated design of the animal feed, and waste treatment process together with the selection of optimal size and location for this type of facility has not been addressed in the literature.

Therefore, this work presents a methodology that aims to simultaneously select the optimal number of animals, the annual crop distribution, the properties of the nutrient recovery process, as well as the location of the facilities. This methodology is implemented through a multi-objective (economic and environmental) and multi-period mathematical optimization model. This model determines the operating costs, income, amount of each crop, and environmental indexes, as well as other data of interest, such as the cost of waste treatment with respect to the cost of meat. Besides, it is generic enough to be easily applied to any set of locations, crops, and animal types. The rest of the paper is organized as follows. In Section 6.2, the methodology is developed including a description of the problem, the reference framework used as starting point, and the main modifications introduced in this work. The solution procedure is also included in this section. In Section 6.3, the model is applied to a case study in Spain and the results are shown. Finally, in Section 6.4, the conclusions are presented.

6.2 FRAMEWORK DEVELOPMENT

6.2.1 *Description of the problem*

This work addresses the integrated design of an intensive beef cattle farm and the cropping system, as well as its location and size, analyzing a set of variables that influence both the environmental impact and economic performance of the farm. The conceptual idea of the integrated system is shown in Figure 6.1.

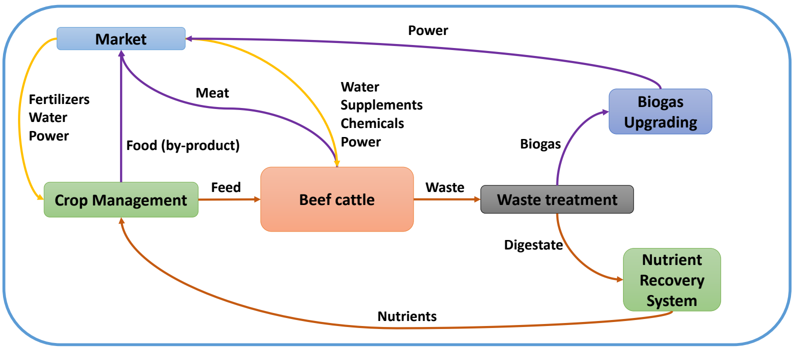


Figure 6.1: Diagram of an integrated system of intensive livestock and cropping system.

The farm is designed to produce the feed necessary to feed the cattle. Therefore, the design of the cropping system is performed by estimating the area needed, for the amount of crop required, using experimental yields. These yields are estimated from technical reports published by governments every year collecting agricultural results and are based on average values (Ministerio de Agricultura, 2019). The amount and type of crop are set by the nutritional and energy requirements of the animals. Several studies have been used to establish experimental relationships between these requirements and the age, weight, sex, and life stage of the animals. This allows estimating the variation in feed composition, as well as crop distribution, throughout the animal's life cycle. These correlations are widely known and can be consulted in the supplementary material. In addition, there are also empirical models that determine the degradation of feed in the digestive process of ruminants (Council, 2000), allowing to estimate the composition of residues as a function of feeding. These correlations, yields, and mass balances have also been included in the supplementary material. The food that is not used as animal feed is sold as a by-product (only barley and wheat since the rest of the crops are either fully fed or have no market value (Taifouris & Martin, 2021)). In addition, the manure is treated to produce biogas and digestate through an anaerobic digestion system. This process is modeled using stoichiometric relationships from the protein, carbohydrate, and lipid composition of the manure, experimental kinetics, and biodegradability yields, following the work of Taifouris and Martín, 2018. Nitrogen, potassium, and phosphorous are recovered using a combined mechanical and membrane separation system. The nutrients recovered are estimated with empirical yields obtained from the literature (Martín-Hernández, 2022). Location is integrated through a series of parameters related to environmental and economic aspects. Some of these are used directly to discard locations (protected areas, nitrate vulnerable zone, natural parks, etc.) while others (crop yields, soil and water availability, land rental prices, etc.) affect the objective function of the optimization model. It is worth highlighting, that the model is multi-objective account for trade-off between the economic and environmental performances. Rather, the model is also multi-period, because the optimization variables are evaluated over 240-time units (20 years).

The solution of this model allows for the simultaneous design of the feed formulation, the waste treatment process, the nutrient recovery system, and the crop distribution, as well as, the location and the size of the facilities.

6.2.2 *Optimization framework*

For the development of the optimization framework, a model from the literature (Taifouris & Martin, 2021), that integrates most of the models described in Section 6.2.1, such as models for estimation of nutritional and energy requirement, crops yield, nutrient recovery and fertilizer consumption, is taken as a starting point. These models are detailed in the supplementary material. Nevertheless, several important modifications are required to account for the selection of the location and to increase the realism of the work of Taifouris and Martin, 2021 . These modifications are the introduction of population groups that grow simultaneously over time, a longer time horizon, a new technology for nutrient recovery, and the integration of the location as a new dimension of the model. The integration of the different locations is expected to increase the size and complexity of the reference model. Therefore, a profound reformulation of the previous models must be performed to solve it.

6.2.2.1 *Integration of the location*

The location is integrated by analyzing the parameters that can affect the operation from economic and environmental points of view. The integration is performed at two levels. On the one hand, a set of environmental constraints (i.e. protected natural areas, nitrate vulnerable zones, and water scarcity) are used to discard locations previously to solve the optimization model. On the other hand, another set of parameters (price, yield, and availability of land and water) is added to the model affecting both environmental and economic objectives. Besides, binary variables are defined to select the location and the type of crops (rainfed or irrigated). In each agricultural district, up to 10 crops (wheat, barley, barley forage, corn, corn forage, oat, rye, sorghum, alfalfa, and vetch) can be selected. Nevertheless, only one of the possible locations is selected.

Thus, the reference framework is converted from nonlinear programming (NLP) problem to a mixed-integer nonlinear programming (MINLP) problem. A large number of locations are expected to be considered, making the model too complex to be addressed directly. Therefore, reformulation is necessary to transform it into a mixed-integer linear programming (MILP) problem. This reformulation is explained in Section 6.2.2.3.

6.2.2.2 *Time horizon and animal population groups*

In the reference work (Taifouris & Martin, 2021), not only the time horizon is limited to 5 years, but also all the animals grew at the same time. In this work, the time horizon is extended up to 20 years, and there are animal population groups, of different ages, growing simultaneously, increasing the realism of the farm model. Each group is formed by those calves that have the same date of birth, constituting a group in which all animals have the same age. It is possible to estimate the age and the number of the animals in each group, as well as the total number of groups as a function of the life cycle of the farm, before solving the optimization model. For this purpose, it is necessary to consider that each cow can have 3 calves and whose births occur in the time unit (TU) 36, 54, 72 of the animal life cycle (Taifouris & Martin, 2021). Females have a life cycle of 72 TU (each TU is equivalent to 24 days to match digester operating time), in contrast to males which are slaughtered in the 22 TU. In the last year of the farm operation, all animals are slaughtered. In addition, it is important to consider that the farm starts with yearlings of 12 TU of age. There are 26 population groups in total along with 20 years. With this information, the groups can be modeled outside of the optimization framework and added as parameters. Therefore, the interval, the number of animals in each group, and the age are known before solving the optimization model. The Gantt chart of different groups can be seen in Figure D.1 in the supplementary material.

The analysis of the animal population groups is important to estimate the animal's requirements and the production of waste per TU. It is necessary to completely reformulate the model to integrate these distributions and to apply all calculations to each population group, considering the time gap between them. To do this, the variables related to nutritional and energy needs, as well as waste production have a new dimension called 'group' (see Sections D.1 and D.2 of the supplementary material). For each group, these variables have a value other than 0 when the time unit of the farm is within the life cycle of that group and 0 otherwise.

6.2.2.3 *Updated estimation of dry matter intake and offline calculation*

The integration of locations, especially in cases where the number of these is high, together with the increase of the time horizon and the integration of population groups, make the model larger and more complex. Thus, it is necessary to reformulate the original model to transform it into a mixed-integer linear programing (MILP) problem. In the reference model, there are several non-linear correlations that complicate the problem. The most important non-linear correlation is used to estimate the dry matter intake per day (DMI). It depends on the weight of the animal and the net energy for maintenance (NEMA) content of the feed (Council, 2000). Since the weight of the animal at the beginning of each of the gestation and calving is fixed through experimental data (Council, 2000), the daily weight gain of the animal is known (see Eq.(D.2)-(D.4) in the supplementary material). Therefore, the weight of the animals in each TU and in each population group can be introduced into the model as a parameter. In the same way, the NEMA of each ingredient is also known (see Table D.6 of the supplementary material). Using this information, it is possible to calculate the DMI per type of ingredient 'j' ($\text{DMIf}_{j,t}$) and per TU 't'. Next, the dry matter intake using the feed ($\text{DMI}_{t,group}$) can be calculated using Eq.(6.1), where $\text{x}_{t,j,group}$ represents the formulation of the feed. This equation is linear.

$$\text{DMI}_{t,group} = \sum_{j} x_{t,j,group} \cdot DMIf_{j,t} \quad \forall \text{t,group} \tag{6.1}$$

In addition, there is a set of variables formed by the total weight and daily weight gain, energy required, the protein required, milk produced (if lactating), and energy consumed in pregnancy (if pregnant) that can be estimated separately from the main model. This is because these variables depend only on the weight of the animal and, therefore, they can be included as parameters. Following these changes, the model is completely linear.

6.2.3 *Solution Procedure*

The solution procedure is performed in two stages. A prescreening and a multi-objective approach to select the feed formulation, crop distribution, size of the farm, and its location.

The prescreening is used to discard those locations that do not meet the following set of environmental restrictions:

- **Protected natural areas**: The agricultural districts where the national park (Ministerio de transición ecológica y de reto demográfico, 2021b), Red Natura 2000 (Ministerio de transición ecológica y de reto demográfico, 2021c), or protected landscape (Ministerio de transición ecológica y de reto demográfico, 2021a) cover an extension of the territory greater than or equal to 50%, are discarded. This percentage was selected because it is assumed that the rest of the area is large enough to locate the farm without affecting the protected area. However, the framework is flexible so that this value can be easily modified without significantly affecting the methodology presented in this work.

- **Nitrate vulnerable zones**: All water bodies that exceed a nitrate concentration of 50 mg/l are considered to be 'Nitrate vulnerable zones' (Ministerio de la presidencia, relaciones con las cortes y memoria democrática, 1996). It is not possible to locate the farm in those agricultural districts where these zones (Ministrerio de transición ecológica y el reto demográfico, 2021) coincide with irrigating crops or where these exceed 50% of districts with rainfed crops.

- **Water scarcity**: The amount of water used for irrigation is limited in each place according to the hydrological plan. By consulting these documents (Ministerio para la transición ecológica y reto demográfico, 2021), it is possible to establish a maximum limit on water consumption. It is assumed that only 1% of the resources currently dedicated to cropping and livestock systems can be used. These limits are established by provinces.

The software 'Arcmap' (Esri, 2015) together with data from the literature presented above are used to represent and estimate the area occupied by the protected and vulnerable zones in each agricultural district. Thus, it is possible to verify whether the agricultural districts meet the constraints.

Once the districts where farms cannot be installed have been filtered out, the next stage which consists of applying the optimization framework over the rest is performed. The solution determines the size of the farm, the best composition of feed, and the location as well as the requirements of cultivation area, the waste treatment, and the nutrient recovery processes. The models that are included in the optimization framework are shown in Figure 6.2. The equations that constitute each of the models can be found in the supplementary material. All these equations are introduced into the optimization model as constraints. Most of them correspond to mass and energy balances, as well as empirical correlations and yields. These models are used to simulate each of the processes described in Section 6.2.1. In addition to the equations, the optimization model requires information on the fertilizer requirement of the crops (Table D.5), nutritional and energy properties of the crops (Table D.6), water availability and price (Table D.8), land rental price (Table D.9), the available rainfed (Table D.10) and irrigated (Table D.11) area. The production yields in both types of land are given in Tables D.12 and D.13. All this information can be found in the supplementary material.

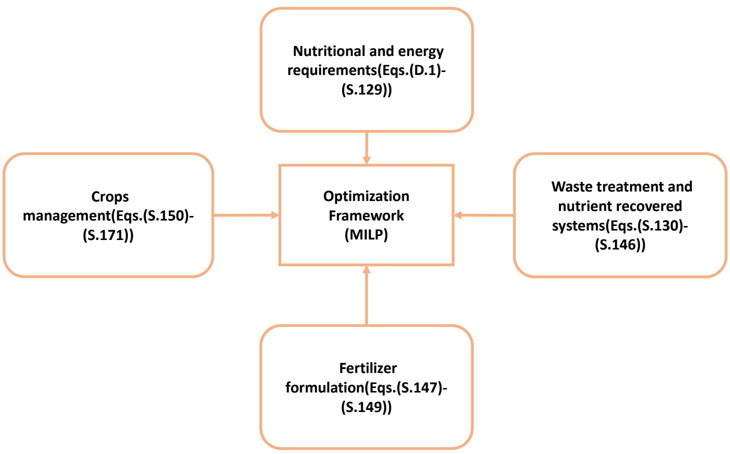


Figure 6.2: Optimization framework

As the optimization framework is multi-objective, the ϵ-constraint method (Mavrotas, 2009) is used to account for both the economic and environmental dimensions of the problem. The objective function used profit (Pro) as an economic indicator (Eq.(6.2)), while the environmental impact is introduced in the model as an additional constraint, limiting its value. This is quantified by simultaneously considering the effect of the farm on the atmosphere, soil, and water consumption, through a composite index that is explained at the end of this section. All prices used in the economic evaluation correspond to the latest annual average prices published in the literature.

$$\begin{aligned}\text{Pro} = \; & In_{Mt} + In_{Crp} + In_{Bio} - Cst_{Crop} - Cst_{Field} - \\ & Cst_{Fertilizer} - Cst_{Storage} - Cst_{Labor} - Cst_{Aux} - Cst_{WasteT}\end{aligned} \tag{6.2}$$

The income from the sale of meat (In_{Mt}) is calculated by analyzing the price of the animal (which depends on sex, age, and weight of animals), the meat yield per animal (Huerta-Leidenz et al., 2013), and the number of animals produced in 20 years (which can be estimated from the procedure shown in 6.2.2.2).

Nutritional models (see Section 6.2.1 and supplementary material) adjust the amount of crop needed for the animals. Nevertheless, it is necessary to generate the entire crop to produce certain ingredients. This is the case for barley or wheat straw, which require producing both straw and grain. If the model does not select both for animal feed, one of them (grain or straw) can be sold. Therefore, 4 types of ingredients (barley straw, barley grain, wheat straw, and wheat grain) are considered for sale, and the model selects the destination of the crop. Income from crop sales (In_{Crp}) depends on the amount of barley and wheat destined to be sold. The rest of the crops are either fed entirely to the animal, or their straw has no market value. As biogas is used to produce power, its heat of combustion (HC), the yield of biogas to produce power (yd), and the price of power (Pr_{power}) are used to estimate its income (In_{Bio}), following Eq.(6.3). The amount of biogas produced can be estimated (Amt_{biogas}) from the waste treatment (see Section 6.2.1 and supplementary material) by using mass balances.

$$\text{In}_{\text{bio}}\text{=Amt}_{biogas} \cdot \text{yd} \cdot \text{Pri}_{\text{power}} \cdot HC \tag{6.3}$$

Regarding costs, they are either estimated using amounts or areas. The cost of land (Cst_{Field}) and labor (Cst_{Labor}) depend on the area cultivated. This is shown in Eq.(6.4)-(6.5).

$$\text{Cst}_{\text{Field}}\text{=} \sum_{l} \sum_{j} \sum_{year} \text{PriS}_{\text{Rent}_l} \cdot \text{AreaS}_{j,l,year} + \text{PriR}_{\text{Rent}_l} \cdot \text{AreaR}_{j,l,year} \tag{6.4}$$

$$\text{Cst}_{\text{Labor}}\text{=} \sum_{j,l,year} \text{Pri}_{\text{MP}} \cdot (\text{AreaS}_{\text{j,l,year}} + \text{AreaR}_{\text{j,l,year}}) \tag{6.5}$$

Where $AreaS_{j,l,year}$ and $AreaR_{j,l,year}$ are the area occupied by crop 'j' (rainfed or irrigated crops) at location 'l' in year 'year'. $PriS_{Rent_l}$ and $PriR_{Rent_l}$ are the rental prices of rainfed and irrigated crop fields, respectively, at location 'l'. Pri_{MP} is the price of labor. These areas are determined according to the amount of crop selected as well as its production yield (kilogram per hectare). The cost of fertilizer ($Cst_{Fertilizer}$), storage ($Cst_{Storage}$), auxiliary costs (Cst_{Aux}), and waste treatment costs (Cst_{WasteT}) depend on the amount of fertilizer needed, crop stored, chemicals used (including water and supplements), and residues treated, respectively. These costs are calculated by Eq.(6.6)-(6.9).

$$\mathrm{Cst_{Fertilizer}} = \mathrm{Amt_N} \cdot \mathrm{Pri_N} + \mathrm{Amt_P} \cdot \mathrm{Pri_P} + \mathrm{Amt_K} \cdot \mathrm{Pri_K} \tag{6.6}$$

$$\mathrm{Cst_{Storage}} = \mathrm{Pri_{storage}} \cdot \left(\sum_{\mathrm{t}} \sum_{group} \mathrm{DMI_{t,group}} \right) \cdot \frac{\mathrm{LC_{farm}}}{\mathrm{LC_{silo}}} \tag{6.7}$$

$$Cst_{Wtre} = \sum_{group} \sum_{t} \mathrm{WAS}_{\mathrm{t},group} \cdot CstUw \tag{6.8}$$

$$\begin{aligned} \mathrm{Cst_{aux}} = {} & \mathrm{Amt_{supP}} \cdot \mathrm{Price_{supP}} + \mathrm{Amt_{supCa}} \cdot \mathrm{Price_{supCa}} \\ & + Cst_{waterAgry} + Cst_{waterLiv} \end{aligned} \tag{6.9}$$

Where Amt_N, Amt_P, and Amt_K are the amount of fertilizer used to provide the nitrogen, phosphorus, and potassium required by the crops selected to produce the feed, and PriN, PriP, and PriK represent their respective prices. $DMI_{t,group}$ is the daily dry matter intake of the animals, LC is the life cycle of the farm and storage facilities, and $Pri_{storage}$ is the storage price. $WAS_{t,group}$ represents the daily amount of waste generated, while CstUw is the unit cost of manure treatment. Amt_{supP} and Amt_{supCa} are the amount of phosphorus and calcium supplements needed to meet the nutritional requirements of the animals. $Price_{supP}$ and $Price_{supCa}$ are the prices of these supplements. $\mathrm{Cst}_{waterAgry}$ and $\mathrm{Cst}_{waterLiv}$ are the cost of irrigation water and the cost of feed water, respectively. These costs are estimated by Eq.(6.10)-(6.11).

$$\mathrm{Cst_{waterAgri}} = \mathrm{CstU_{waterAgri_l}} \cdot \mathrm{CAA}_j \cdot AreaR_{l,j,year} \tag{6.10}$$

$$\mathrm{Cst_{waterLiv}} = \mathrm{Wa_{Animal}} \cdot \mathrm{NA_{Animals_{group}}} \cdot \mathrm{lt_{Animal}} \tag{6.11}$$

Where $\mathrm{CstU}_{waterAgri_i}$ is the unit price (€/m^3) of irrigation water, CAA_j is the annual water consumption of the crop 'j' and $\mathrm{AreaR}_{l,year}$ is the cultivation area of the crop 'j' in the region 'l' en the year 'year'. Wa_{Animal} is the water consumption of the animals (calves, yearlings, or cows), $\mathrm{NA}_{Animal_{group}}$ is the number of each type of animal in each group, and lt_{Animal} is the lifetime of each animal. Cst_{Crop} is the cost associated with feeding the animals (only tillage, sowing, and harvesting of the used crops) to grow the animals from birth to slaughter. This cost is estimated by Eq.(6.12).

$$\mathrm{Cst_{Crop}} = \sum_{group} \sum_{t=1}^{t=240} \mathrm{DMI_{t,group}} \cdot \mathrm{Cst}_j \cdot x_{t,j,group} \cdot \mathrm{NA_{animal_{\mathit{group}}}} \tag{6.12}$$

Where Cst_j is the cost of production of each crop and $\mathrm{NAanimal}_{group}$ is the number of animals (calves, yearlings, or cows, depending on the life cycle of the animal) in each group. The number of animals in each group can be estimated following the procedure shown in Section 6.2.2.2. $x_{t,j,group}$ is the fraction of the crop 'j' in the DMI for each TU 't' and for each group.

These costs, as well as the previous ones are fixed by the size of the farm, its location, and crop selection. To meet specific nutritional requirements, which are set by the model explained in Section 6.2.1 and shown in the supplementary material, different crops (type and amount) can be used. They consume different amounts of fertilizer (see Table D5 of the supplementary material) and have different production yields (see Table D12 and D13 of the supplementary material) determining the area occupied. The composition of the selected crops does not only affect the amount and composition of the residues, but also the amount of supplement to be added. Therefore, the determination of both costs and income is carried out in conjunction with the rest of the models explained in Section 6.2.1 (see Figure 6.2). The procedure for the calculation of each of these terms is explained in detail in the supplementary material (Eqs.(D.172)-(D.191)).

Regarding the environmental impact, a composite index (CI) is presented to estimate the impact of the facility on the atmosphere (global warming potential (GWP)), soils and water bodies (eutrophic potential (EUi)), as well as the water footprint (WF) of both animals and crops. This is introduced into the model through Eq. (6.13).

$$\mathrm{CI} = \sum_{x} \omega_x \cdot In_x \quad \forall \mathrm{x} \;\; \mathrm{x} \in \{\mathrm{GWP,EUp,WF}\} \tag{6.13}$$

Where ω_x is the weight of each contribution and In_x are the normalized indexes. These weights are estimated based on the literature (Sala & Cerutti, 2018) and the indexes are standardized, with the min-max method

(OECD & Commission, 2008) using Eq. (6.14). The unit value ($Iu_{x,f}$) of the indexes 'x' for each type of fertilizer 'f' can be found in Table D.2 of the supplementary material. The indexes corresponding to the GWP and EUi are calculated by Eq. (6.15), while the index corresponding to WF is calculated by Eq (6.16).

$$In_x = \frac{I_x - min(I_x)}{max(I_x) - min(I_x)} \quad \forall \text{x} \in \{\text{GWP,EUp,WF}\} \tag{6.14}$$

$$\begin{aligned} I_x = \sum_f (Iu_{x,f} \cdot AmtF_f) \ \ \forall x \in \{GWP, EUp\}, \\ \forall f \in \{NH_4NO_3, Ca(H_2PO_4)_2, K_2SO_4\} \end{aligned} \tag{6.15}$$

$$I_x = \sum_j (A_j \cdot AmtUW_j \ \ + AmtC_j \cdot WFC_j) \ \ \forall \text{j} \text{ ,x} \in \{\text{WF}\}, \tag{6.16}$$

Where $AmtF_f$ and $AmtC_j$ are the amount of each type of fertilizers 'f' and crops 'j', respectively. $AmtUW_j$ is the amount of water per unit of area of each irrigated crop 'j' and WFC_j is the water footprint of each rainfed crop 'j' (see Table D.5 and D.3, respectively, in the supplementary material). For more details on the evaluation of the indexes and their integration into the model, see the supplementary material.

6.3 RESULTS

The methodology described in Section 6.2 is applied to a case study formed by 345 locations, corresponding to the agricultural districts in Spain. They can be seen in Figure 6.3.

First, the prescreening discards the agricultural districts following the constraints described in Section 6.2.3. A total of 145 districts are discarded. Subsequently, the multi-objective approach determines the size of the facility, its location, and the crop distribution by looking for a trade-off between economic profit and environmental impact. At this point, the distributions of crops and animals are also analyzed to establish relations between them. The model is an MILP with 6 million equations and 5.3 million variables (36 thousand binary variables). It is solved using CPLEX (GAMS) in an Intel Core i7-7700 computer at 3.6 GHz.

6.3.1 *Selection of the size and location of the farm*

A sensitivity multi-objective analysis is performed to determine the optimal initial number of animals and the farm location. Profit is used as

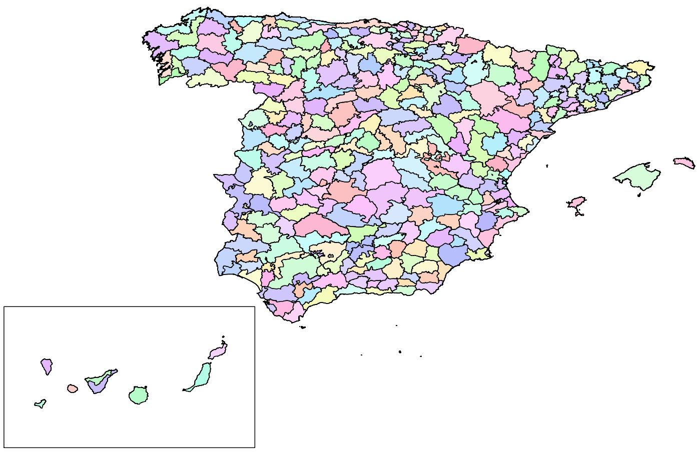


Figure 6.3: .-Agricultural districts in Spain

an economic indicator and the composite index as an environmental impact indicator. Therefore, the variation of profit for different values of CI, farm size, and locations are analyzed and shown in Figure 6.4. It is assumed that up to 10% of the total available area in each agricultural district can be used. This value was set so there is sufficient area for an intensive livestock facility (more than 1000 animals living in the facility) and at the same time be a conservative and realistic value. However, this value can be easily changed depending on the specific characteristics of each case study. The composite index is calculated by using of minimum value of GWP, EUi, and Waterfootprint of the smallest facility of each location and the maximum values of these indexes of the largest possible facility in each agricultural district. After applying the optimization, there are 3 locations suitable for the installation of the farm, 'Campiña','Bureba-Ebro', and 'Campos'.

In addition, the crop production is also evaluated against the initial number of animals (Figure 6.5) to determine the reason for the difference in profit and composite index between the locations considered.

Figure 6.4 shows that 'Campiña' is the best option with respect to profit when the number of initial animal units is small (less than 450), while the district 'Campos' is the only option when the number of animals is larger than 1400. 'Bureba-Ebro' is the district with the highest profit from 500 animals, but it has a size limit of 1400 animals. From this point, the area of cultivation to produce feed is insufficient and this district cannot be chosen.

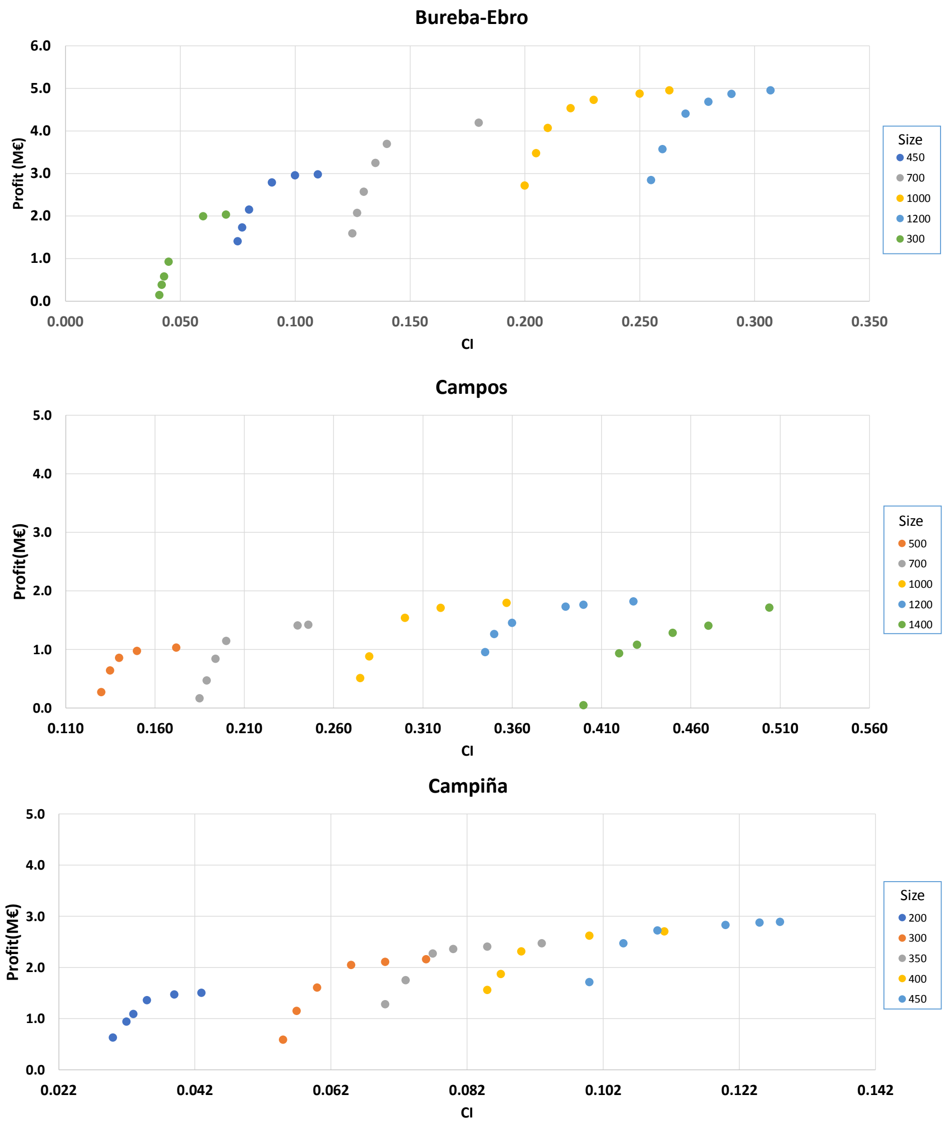


Figure 6.4: Multi-objective analysis of locations and sizes of the facility

'Bureba-Ebro has the point of highest possible profit considering all the agricultural districts (i.e 1200 initial animals). However, analyzing profit together with the composite index of environmental impact, it can be observed that there are points with similar profit but with a larger difference in the value of CI. For instance, the point corresponding to 1200 animals, with a composite index of 0.307, has a benefit of 4.95M€, while in the case of 1000 animals, there is a scenario with a similar profit (only 1.6% lower) but with an environmental impact 18.56% lower. The same occurs with other points corresponding to the cases of 1000 and 1200 animals.

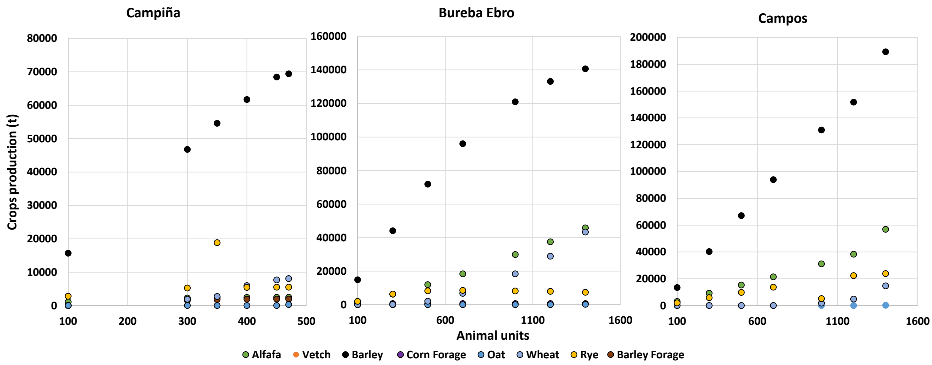


Figure 6.5

Figure 6.6: Crop production as a function of the number of animals for the three best locations

Nevertheless, in the rest of the scenarios, the points are farther away from each other. For this reason, it is considered that the size that best balances both objectives (economic and environmental) is the initial 1000 animals.

By analyzing Figure 6.5, it confirms that the main crop is barley for the three agricultural districts. In addition, this crop is also the most produced for any size of farm. Therefore, those districts that have a higher yield to produce this crop have lower operating costs and lower environmental impact to produce the same amount of barley. Of the three districts considered, 'Campiña' and 'Bureba-Ebro' have a similar yield to produce barley straw (see Table D.13 of the supplementary material). However, this yield in 'Campos' is 1.52 times lower than in 'Bureba-Ebro' and 'Campiña' (1.8 t/ha vs 2.8 t/ha). This means that an increase in the cultivation area is required to produce the same amount of barley, which in turn results in an increase in the costs related to the area and fertilizer consumption. This explains the large difference in profits between this location and the others. The difference between 'Campiña' and 'Bureba-Ebro' lies in the cost of the land, being 2.63 times cheaper in 'Campiña' (see Table D.10). In addition, since barley straw is a key ingredient for animal feed, its availability limits the selection of districts. 'Campiña' can only handle up to an initial number of animals of 470 since its available area is 1.41 times lower than 'Bureba-Ebro' for barley ($1.8{\cdot}10^4 ha/year$ vs $2.6{\cdot}10^4 ha/year$), 1.7 times for rye ($5.7{\cdot}10^2 ha/year$ vs $9.7{\cdot}10^2 ha/year$), and 6.92 times for wheat ($5.2{\cdot}10^3 ha/year$ vs $3.6{\cdot}10^4 ha/year$), which are the three main crops following the Figure 6.5. However, 'Campos' can be selected for an animal's number of 1400 since it is the district with the highest availability of barley crops, 3.4 times higher than Bureba-Ebro ($6.1{\cdot}10^4 ha/year$ vs $1.8{\cdot}10^4 ha/year$).

Currently in Spain, one of the most important intensive livestock farms is in 'Caporroso' (Muñoz, 2021)(a municipality in the agricultural district of 'Ribera Alta Aragón'). If the methodology described in this work is applied, this location would have been discarded beforehand in the prescreening because it is a nitrate vulnerable zone. In addition to this installation, two more are in the planning stage, one for the municipality 'Torralba de Aragon' (Villanueva, 2021)('Monegros') and another for the municipality of 'Noviercas' (Villanueva, 2020) ('Campos de Gomara'). 'Noviercas' does not exactly coincide with a nitrate vulnerable zone but it is very close (less than 10 km) so the procedure would also discard it. The only location that would pass the prescreening would be 'Torralba de Aragon'. However, 'Monegros' is a district with a lower yield (3.82 times) in barley straw than 'Bureba-Ebro' (2.8 t/ha vs 0.73 t/ha), so the cost of production would increase (as it would require more cultivation area) and income would decrease (as there would be less grain to sell).

'Caporroso', 'Torralba de Aragon', and 'Noviercas' are 3 examples of intensive livestock farms decoupled from crop systems. However, it has been demonstrated in previous works (Taifouris & Martin, 2021), that the integrated development of both sectors can reduce the environmental impact by up to 65% (compared to the uncoupled systems). This impact can be further reduced by considering the environmental properties of the place where it is implemented, as is done in the prescreening stage of this work. This would contribute to reducing the negative image that these facilities have (Armestre, 2021) due to the improper treatment of waste and animals.

6.3.2 *Multi-objective techno-economic analysis*

Once the size and location are fixed, the Pareto curve corresponding to the size of 1000 initial animals for the "Bureba Ebro" location is analyzed. This curve could be analyzed directly in Figure 6.4 , however, the limits used to normalize the environmental impact indexes (see Section 6.2.3) must be updated, since they were calculated considering different farm sizes (the minimum values of each index corresponded to the smallest sizes and the maximum values to the largest sizes). For this new Pareto curve, the values of the composite index consider only scenarios of a farm of 1000 initial animals. The minimum values of GWP, Eui, and WF correspond to the scenarios that minimize each of these indices, while the maximum values correspond to the scenario in which profit is maximized, without considering the environmental impact. These values are shown in Table D.4 of the supplementary material. For this reason, the values of the composite index are different from those shown in Figure 6.4. The new Pareto curve is shown in Figure 6.7. 3 scenarios of interest are highlighted. First, a scenario is considered in which no environmental constraint is introduced in the model, resulting in the economic optimum. A second scenario that minimizes the environmental impact of the economic activity is evaluated. Finally, the scenario that best balances the two objectives is also considered. A techno-economic study is carried out for each scenario and the results are presented in Figure 6.8.

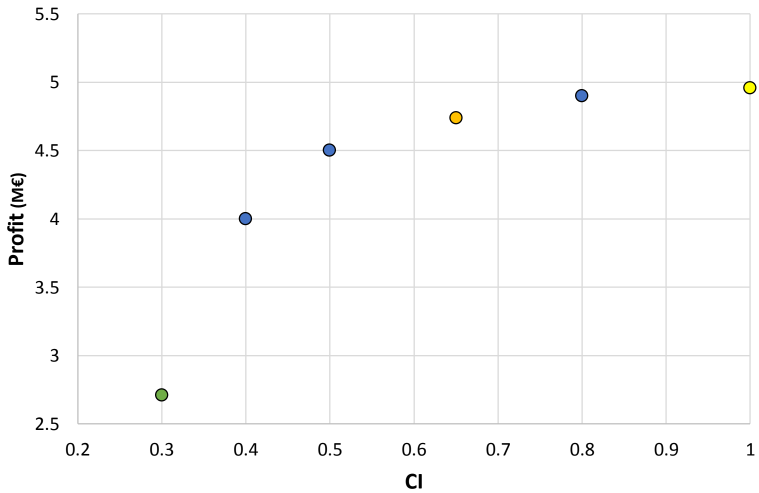
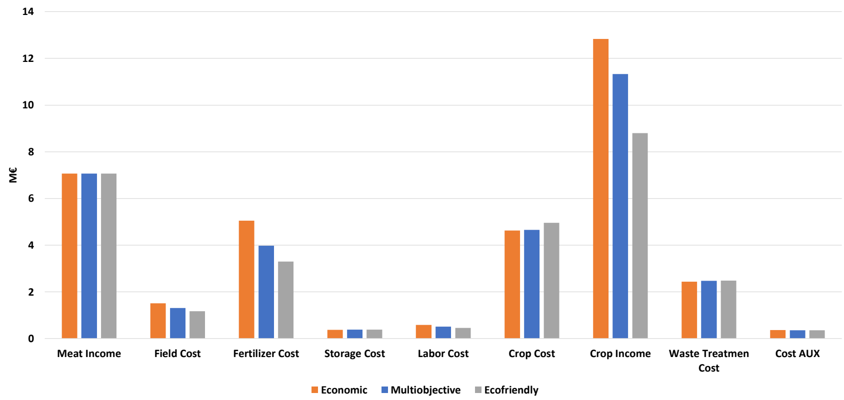


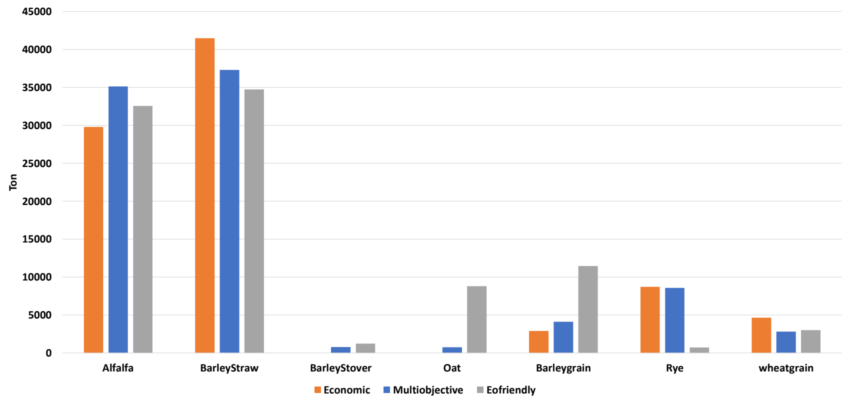
Figure 6.7: .-Relation between composite index and profit (Economic: yellow, Multi-objective: orange; Ecofriendly: green)

The profits of the economic, multi-objective, and eco-friendly scenarios are 4.9M€, 4.7M€, and 2.7M€, respectively. While the composite indexes are 1, 0.65, and 0.3 for the economic, multi-objective, and eco-friendly scenarios, respectively. Between the economic and multi-objective cases, the composite index drops 35%, while the profit only drops 0.22M€ (4.4% lower). Nevertheless, if the multi-objective scenario is compared with the eco-friendly case, the composite index drops 0.35, but the profit drops 2.03M€. For this reason, the multi-objective scenario is postulated as a trade-off between economic and environmental objectives.

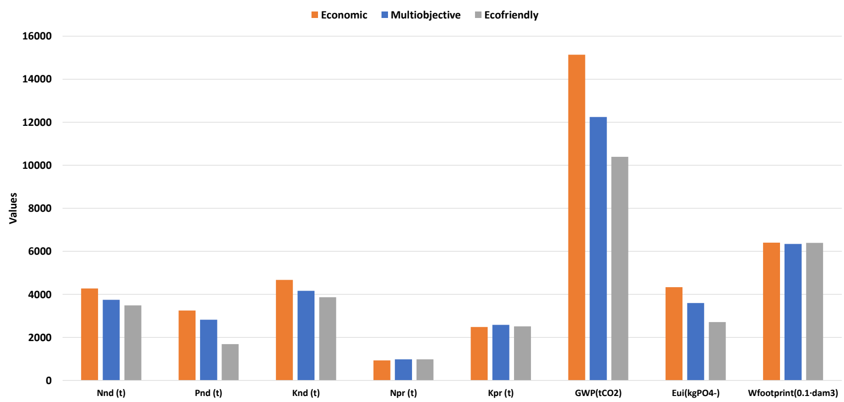
Concerning income, all scenarios show a higher income from crop sales than from meat sales (see Figure 6.8a). This means that cropping is the most profitable economic activity. Nevertheless, the central activity is sought to be the livestock and, therefore, the commercial management of crops is limited and oriented to animal feed. The income from the sale of



(a) Economic analysis



(b) Analysis of crop production for animal feed



(c) Environmental analysis and nutrient balance (Nd:needed and Rc:recovered)

Figure 6.8: Tecno-economic analysis for economic, multi-objective and eco-friendly scenarios.

power produced using the biogas generated from waste treatment has not been included in Figure 6.8a because it represents less than 0.05% of the total income in all scenarios.

Regarding costs, the most important are fertilizer costs, crop costs (which include tillage, sowing, and harvesting), and waste treatment costs. The cost of the water used as feed is especially low because water is cheap. This is because hydrological plans (Ministerio para la transición ecológica y reto demográfico, 2021) have been used to estimate the cost of using water from an existing water source (rivers, lakes, etc.). It can be seen that the cost of waste treatment is similar in the three cases (over 2.5M€). This is due to the fact that this cost is estimated based on the amount of waste generated. Although its composition varies from one scenario to another, its amount is similar.

Another important result is the comparison between the cost of meat production and the consumer benefit (CB). The CB is 1 kg of consumed, boneless, edible beef and is calculated corresponding to 29% of the live weight (Asem-Hiablie et al., 2019). In the course of the 20 years of operation of the farm, 5305 tons of meat are generated, considering both yearlings and cows slaughtered. The CB is 1538 tons. The cost of meat production is 8.87 €/CB (of which 1.61 €/CB corresponds to the cost of waste treatment) for the multi-objective case. This cost is similar to the selling price of meat in Spain (9.84 €/CB (Statista, 2021)). Nevertheless, this price includes other economic items, such as packaging, transportation, and profit margin, which are not considered in this work. However, the meat cost of this work can be reduced, if it is considered the income from the crops sold, down to 1.51 €/CB.

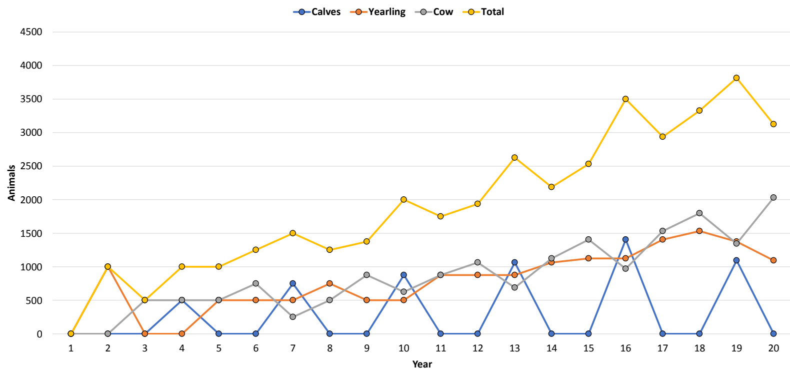
The decrease in profit between the economic and the multi-objective scenarios is due to the decrease in the amount of barley straw (see Figure 6.8b), which is replaced by other crops with higher yields (larger amount per hectare), such as alfalfa and vetch, to reduce the cultivated area, and therefore, the consumption of fertilizer. In addition, a significant amount of the barley grain produced (which was destined for the food market in the economic scenario) is also devoted to animal feed, reducing the need for wheat or barley straw, as can be seen in Figure 6.8b. Nevertheless, these changes do not only reduce the environmental impact of the facility (19% lower in GPW and 17% lower in EUi) but also the amount of barley grain available for sale, and thus, the income from crops. However, this is mitigated by economic savings in fertilization, labor, and soil costs since the total cultivated area is 10% lower. However, when comparing the multi-objective scenario with the eco-friendly scenario, it is observed, in Figure 6.8a, that the economic savings in fertilizer do no longer compensate for the reduction in income from crop sales. In this case, it is very difficult to further reduce the area needed through changes in the selection of the crops. Therefore, efforts are concentrated on increasing the amount of barley grains devoted to animal feed by 2.79 times compared to the multi-objective scenario, as can be seen in Figure 6.8b. This allows a 6% reduction in the total cultivated area since the amount of alfalfa, barley straw, and rye are reduced but causes a sharp drop in profits. The reduction in environmental impact is concentrated on reducing GPW by 15% and Eui by 25% as can be seen in Figure 6.8c.

Regarding the environmental impact indexes, it can be observed that the WF is similar in the three scenarios (see Figure 6.8c), with the use of rainwater (green water footprint) being much higher than the artificial input from rivers, lakes, and groundwater sources (blue water footprint). This is because irrigated crops are not used in any of the 3 scenarios. While the green water footprint of the facility is slightly higher (9370 m^3/t vs 8849 m^3/t) than what can be found in the literature, the blue water footprint is much lower (Mekonnen & Hoekstra, 2012). Nevertheless, the water footprint depends on the technology and weather of countries since there are some countries, such as Brazil or China, that can have a water footprint larger than $8000 m^3$ per ton of meat, while that others like the United State or the Netherlands does not exceed 5000 m^3/t (Gerbens-Leenes et al., 2013). Finally, with respect to GWP, it is observed that the results obtained in the ecofriendly, multi-objective, and economic scenarios (1.96, 2.31 and 2.85 $kgCO_2/kg$ live weight, respectively) are slightly lower than those reported by the literature (Pelletier et al., 2010; Roop et al., 2014). According to these work, GWP varies from 3.47 $kgCO_2/kg$ live weight to 5.59 $kgCO_2/kg$ live weight depending on the type of crop, the type of animal, as well as the age, and weight at the time of slaughter. The numerical data of this Section can be consulted in Table D.7 of the supplementary material.

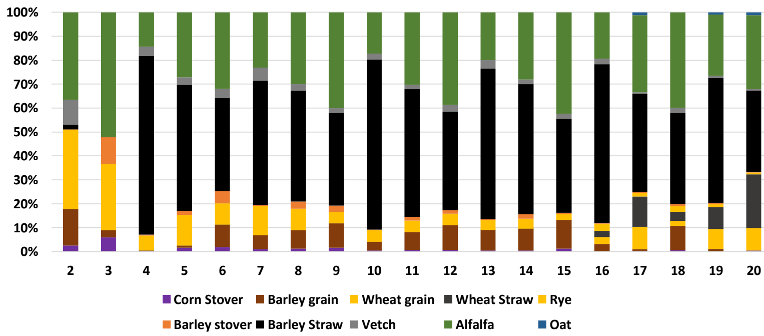
Finally, analyzing the nutrient balance, it is determined that, for the multi-objective case, it is possible to recover the 26.2% of nitrogen and 62% of potassium necessary for crop growth. The nutrient requirement of the multi-objective scenario is 12% less than in the economic scenario. Whereas, if this scenario is compared to the eco-friendly scenario, the nutrient requirement is 15.7% higher.

6.3.3 *Animal and crop distribution for the multi-objective scenario*

The distribution of animals through the farm operation is analyzed together with the percentage of each crop needed per year. This study is shown in Figure 6.9. The joint representation of animals (Figure 6.9a) and crop distribution (Figure 6.9b) allows relating changes in crops to the number and age of the animals along the life cycle of the farm.



(a)



(b)

Figure 6.9: Animal (a) and crop distribution (b) along the life cycle of the farm

First, during year 1 there are no animals on the farm, so the crop distribution in year 2 is grown, harvested, and stored during year 1 to feed the animals in year 2. Therefore, the crop distribution shown in Figure 6.9b of a specific year corresponds to the feed needed for the animals of that year yet is planted and harvested in the previous year. Thus, the crop and animal distributions can be directly compared year by year. It is observed that in the first years (i.e., years 2 and 3), almost 50% of the crops are concentrated (wheat and barley grains). This is due to the type of animals during theses years are only yearlings (12- month-old) and young cows. They need more concentrate than forage because the dry matter intake (DMI) of this kind of animals is low and needs more energetic ingredients.

Between years 4 and 6, the main changes affect the barley straw and alfalfa fraction. This year 4, there are cows and calves, yet the largest proportion of the total DMI belongs to cows. In this year, cows are 48-month-old and at this age, the energy requirements are low. For this reason, the fraction of barley straw is much higher than that of alfalfa since its NEMA is lower than the NEMA of alfalfa (0.6 Mcal/kg vs 1.24 Mcal/kg). Nevertheless, from year 5, the population of yearlings is older which affects crop distribution. Cows start eating less feed and yearlings more. In addition, yearlings need more energetic forage than cows. As a result, the fraction of alfalfa is larger than in year 4. In year 6, both yearlings and cows continue to grow and, consequently, cows have a lower DMI, and yearlings have a higher DMI. This results in a larger fraction of alfalfa in the crop distribution for the same reason as the previous year.

However, there is a change in trend in year 7. The number of cows decreases, yearlings are older, and the number of calves increases. In this situation, the DMI is adjusted for the needs of the yearling. However, these yearlings are older and require less energy, increasing the fraction of barley straw, restarting the loop (see Figure 6.9b). It is possible to see 5 crop distribution periods since the animal distribution is cyclical every 3 years. Nevertheless, in the two last years (i.e. years 19 and 20), due to the beginning of the dismantling process of the farm, the distribution of animals changes, which slightly breaks the periods, significantly increasing the amount of wheat straw. This is due to the abrupt drop in the number of yearlings. These results are consistent with previous work (Taifouris & Martin, 2021).

6.4 CONCLUSION

This work presents a methodology for the simultaneous design of products, processes, and location for an integrated system of intensive livestock and crop management, which consist of a two-step procedure. Following this methodology it is possible to systematically select the best feed formula (and with it the necessary crops year by year), establish the raw materials and products obtained from the waste treatment and design the nutrient recovery process, as well as determine the best possible location and size, all from an economic and environmental point of view. For this purpose, a multi-objective and multi-period optimization model (MILP) is developed and applied to a case study in Spain.

From the results of the prescreening stage, 42% of the initial locations available do not meet the environmental constraints, demonstrating the importance of carrying out a preliminary analysis to study the viability of the locations considered.

The results of the multi-objective approach show that the optimal location is closely related to the size of the farm, finding the best value of 1000 initial animals in the agricultural district of 'Bureba-Ebro', from economic and environmental point of view. The benefit achieved with this selection is 2.78

times higher than the second-best option, 'Campos'. This demonstrates the importance of considering location and farm design simultaneously.

Once the facilities are placed in Bureba-Ebro and its size is fixed to 1000 initial animals, the selection of the crops (type and quantity) necessary to satisfy the nutritional needs of the animals is analyzed, readjusting the composite environmental impact index and proposing 3 scenarios, economic, multi-objective and eco-friendly. This study shows that, when comparing the multi-objective scenario with the economic scenario, a very significant reduction of the environmental impact (35%) of intensive livestock farming is possible by selecting crops with a higher yield per hectare (alfalfa and vetch) and orienting the production of barley grains to animal feed instead of sending them to the market. This reduces the total crop area, and therefore, the total nutrient consumption (12%). However, this also implies a reduction in profits (4.4%) that can be compensated by incentive policies oriented to the creation of sustainable processes (Martín-Hernández et al., 2022). Since crop yields depend on the location of the facilities, the consideration of location in this type of problem is key for holistic optimization.

It is important to highlight that the most profitable economic activity is crop production (representing between 55% and 65% of total revenues depending on the scenario considered). This opens the possibility of orienting this type of integration to crop production, with meat being a by-product of the facility, and comparing it to the approach presented in this work. In addition, power production through biogas does not represent an important source of income and the most important costs are those associated with crops (34.10%), fertilizer (29.11%), and waste treatment (18.13%) in the multi-objective scenario. Finally, it is possible to reduce the cost to produce meat by 82.9% by considering the incomes of the crops as a method of reducing costs.

Regarding crop distribution, it should be noted that, except for the first years, the most important crops are alfalfa and barley (straw). The variation in the fraction of each of these two crops depended on the number, age, and type of animals predominant each year, forming a total of 5 loops where the crop distribution is repeated with the animal distribution.

6.5 ACKNOWLEDGMENTS

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Part II

ADDED-VALUE PRODUCTS FROM WASTE VALORIZATION

7

INTEGRATED DESIGN OF BIOREFINERIES BASED ON SPENT COFFEE GROUNDS

ABSTRACT

The circular economy concept applied to the management of spent coffee grounds (SCG) is an opportunity to obtain a portfolio of high added-value products and reducing the environmental impact while increasing the profitability and reducing the energy consumption of the soluble coffee production process. A systematic analysis of the alternatives is performed to unveil integration opportunities and find synergies aiming at the optimal set of processes and products. In this work, five products, dry natural extract, dry natural pigment for the textile industry, biogas, digestate, and electrical energy, through three different processes are considered. The use of SCG to produce biodiesel is discarded after prescreening. A systematic techno-economic analysis of all processes is carried out, and two processes were found economically promising, the production of power and the production of natural extract and pigment. The production of natural pigment and natural extract is the most profitable process, with a profit 40 times larger than the production of electrical energy. The operation and investment costs are 4.59 MM€/year and 13.97 MM€, respectively. Therefore, it is possible to achieve economic benefit from the treatment of this waste.

Keywords: Sustainable design, waste valorization, food waste, coffee grounds.

RESUMEN

El concepto de economía circular aplicado a la gestión de los posos de café (SCG, por sus siglas en inglés) es una oportunidad para obtener una cartera de productos de alto valor añadido y reducir el impacto ambiental, al mismo tiempo que se aumenta la rentabilidad y se reduce el consumo de energía en el proceso de producción de café soluble. Se realiza un análisis sistemático de las alternativas para descubrir oportunidades de integración y encontrar sinergias con el objetivo de obtener el conjunto óptimo de procesos y productos. En este trabajo, se consideran cinco productos, extracto natural, pigmento natural para la industria textil, biogás, digestato y energía eléctrica, a través de tres procesos diferentes. El uso de SCG para producir biodiesel se descarta después de la preselección. Se lleva a cabo un análisis técnico-económico sistemático de todos los procesos y se encontraron dos procesos económicamente prometedores: la producción de energía y la producción de extracto y pigmento natural. La producción de pigmento y extracto natural son los procesos más rentables, con una ganancia 40 veces mayor que la producción de energía eléctrica. Los costes de operación e inversión son de 4,59 MM€/año y 13,97 MM€, respectivamente. Por lo tanto, es posible obtener beneficios económicos del tratamiento de este residuo.

Palabras clave: Diseño sostenible, valorizacion de residuos, residuos alimentarios, posos del cafe

7.1 introduction

Society faces three problems: energy, food, and reducing the high production of waste. The three represent not only a demand, supply, and management issue, but they also show a large environmental impact, which is increasingly aggravated due to the growth of the world's population. In particular, the effect of uncontrolled waste production represents already a challenge, and society is becoming aware and concerned. As a result, more restrictive legislation on waste generation is being approved (European Commission, 2020), favoring the development of a circular economy and the bioeconomy. The main idea is to valorize the waste generated in a biological process into high added-value products that are used as raw materials for other industries or are directly sold to the final consumer (European Commission, 2020) . Some examples of added-value products that can be obtained from waste are essential oils (Bustamante et al., 2016; Criado & Martín, 2020) and natural extracts (Brazinha et al., 2015). The bioeconomy concept applied to the food industry has not only economic benefits such as the creation of direct and indirect jobs and the improvement of the competitiveness of production processes but also environmental benefits (Criado & Martín, 2020). Among the products of the food industry, one stands out above the rest, coffee. Coffee is the second most important consumer product after oil (Murthy & Naidu, 2012) with a production of 10.16 billion kilograms between 2018 and 2019 (Organization, 2020). Its production is mainly concentrated in countries such as Brazil, Vietnam, Colombia, Indonesia, Ethiopia, India, and Honduras, with Brazil being the largest coffee exporter in the world (Rajesh et al., 2020). In the production of coffee, a large amount of waste is generated, especially the spent coffee grounds (SCG) and the coffee silver skins (CSS) (Murthy & Naidu, 2012) . In the coffee industry, 650 kg of SCG per ton of green coffee beans and 2 kg per kilogram of soluble coffee produced are generated (Rajesh et al., 2020).

In the countries mentioned above, current environmental laws are more permissive than in the case of Europe or the US, so this type of waste ends up in landfills, incinerated, or used as compost. This causes a series of environmental problems such as soil contamination (Cruz et al., 2012), due to the presence of toxic substances such as caffeine or other polyphenols, the production of greenhouse gases such as $CH4$ and CO_2, due to the decomposition of organic matter, and the release of large amounts of CO_2 in incineration processes. Alternatively, SCG can be used to produce a wide variety of high added-value products due to its composition. The use of the residue to produce these high added-value products does not only reduce its environmental impact but provides additional value, closing the life cycle, transforming the waste from one industry into the raw material for another, pursuing the goal of zero-waste emissions leading to a truly circular economy by closing the life cycle. Some authors have studied the use of SCG to produce different types of biofuels, such as biodiesel and bioethanol,(Kondamudi et al., 2008; Kwon et al., 2013) biogas, (Vítěz et al., 2016) bio-oil (Ktori et al., 2018), and pellets (Kamil et al., 2019); food supplements and biocomponents for the pharmaceutical and cosmetic industries, such as caffeine, antioxidants, and phenolics (Shi, 2016); natural extracts (Ribeiro et al., 2013; Brazinha et al., 2015); additives for industry, such as tannins (Low et al., 2015) or polymers such as polyhydroxyalkanoates (PHAs) (Obruca et al., 2014) ; fertilizer production for some types of crops (Liu & Price, 2011) and energy production (Ciesielczuk et al., 2015) . However, these are experimental studies that only evaluate the production yields of various products but do not carry out techno-economic studies of the entire process. In addition, techno-economic analyses are focused on the production of specific products (Mussatto et al., 2013; Brazinha et al., 2015). The use of SCG for the production of added-value products represents an opportunity to reduce the environmental impact of the coffee industry, reducing the energy consumption and waste generation, while improving its economics. The selection of the portfolio of products requires a systematic analysis of the alternatives to unveil the synergies and integration opportunities.

In this work, mathematical optimization techniques are used for the design of a process that transforms the SPG into a portfolio of products including high-added-value ones. The treatment of coffee wastes must be economical and environmentally conscious and with the final aim of integrating this process as a section of a soluble coffee production plant, favoring the circular economy. Five products, dry natural extract, natural pigment for the textile industry, biogas, digestate, and electrical energy, and three processes are considered. On the one hand, the spent coffee ground extract shows interesting values of phenolic compounds such as caffeine and chlorogenic acids that show antioxidant and antitumor activity (Esquivel & Jiménez, 2012). Furthermore, caffeine is related to the decrease in depression,(Lucas et al., 2011) fatty liver, and other diseases (Molloy et al., 2012). On the other hand, the use of natural pigments in the textile industry can increase the safety of the dyeing process due to the low toxicity of this pigment and the increased sustainability in terms of chemistry and energy consumption. Most of the pigments and natural extracts are obtained from vegetable or animal sources (Bechtold et al., 2003) requiring cultivation or harvesting of the natural environment in which they are produced, causing a negative environmental impact. The natural extracts and pigments obtained from waste do not only reduce the environmental impact of the process in which they are generated but also represent a valorization of the waste promoting circular economy. The digestate obtained from the SCG can be used as a natural fertilizer and substitute part of the mineral fertilizer used for the production of coffee beans. All of the products that can be obtained from the SCG do not compete for part of the market but rather replace part of the current products with others with a more sustainable origin and favor the circular economy of a process with high environmental impact.

This work corresponds to the conceptual level design of the facility, constituting a previous step to the design and construction of a biorefinery providing a guide toward the use of SCG. The rest of the paper is organized as follows. In Section 7.2, the mathematical optimization model is developed, including the modeling of the processes with the energy and mass balance, considerations, and diagrams. An economic analysis is carried out as well. In Section 7.3, the model is applied for a representative industrial case, and the results are presented, and in Section 7.4, the conclusions are discussed.

7.2 PROCESS DESCRIPTION

In this Section, the superstructure of alternative processes is described, shown in Figure 7.1.

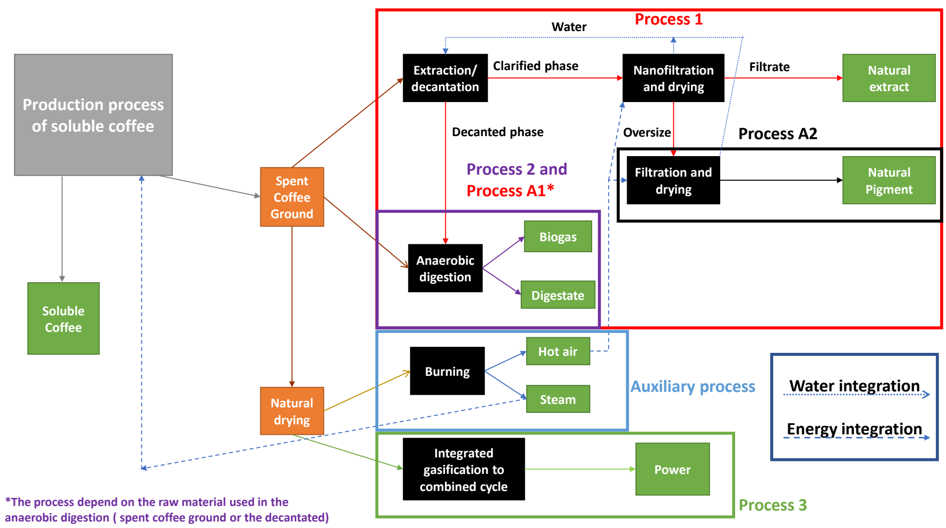

Figure 7.1: Superstrucure for the use and integration of spent coffee grounds.

Three main processes and two subprocesses derived from Process 1 (Process A1 and Process A2) are considered for the valorization of the

SCG. The modeling of the processes is carried out using mass and energy balances, phase equilibria, experimental yields, and rules of thumb to describe the yield and performance of each one of the units (Martin, 2016). Process 1 consists of an extraction-filtration system for the production of a natural coffee extract of high added value. This process generates two residues that are valorized through anaerobic digestion (Process A1) to produce biogas and digestate and a drying process (Process A2) to produce natural pigment. Process A1 and Process 2 use the same technology, but the difference is the raw material. SCG is used as a raw material for Process 2, while Process A1 uses the residue from the decanter of Process 1. Finally, Process 3 uses the SCG to produce electrical energy using a gasifier and a combined cycle. The processes are modeled following an equation-based approach in GAMS.

In the design of the superstructure, the integration of energy and water is considered (see Figure 7.1). The energy required for the anaerobic digestion, filtration, and drying processes is generated within the facility through an auxiliary process. The processes that require dry raw material are discarded due to the cost of energy involved in the drying stage of raw material with 60% humidity. The composition of the raw material is shown in Figure 7.2.

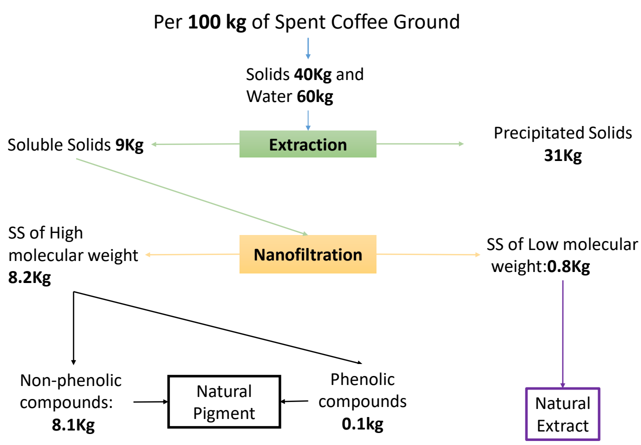

Figure 7.2: Composition of the spent coffee grounds.

This composition is obtained from the mass balances shown in the literature (Brazinha et al., 2015). In addition, another important piece of information to model the mass balances is the average density of the solids of the SCG. Given the density of the SCG and its water content (Telis-Romero et al., 2000), the average density of the solids is determined (1.329 kg/dm^3). Besides, the density of citric acid (ρ_{ac}) is 1.66 kg/dm^3 (Lide, 2005; Criado & Martín, 2020). In that work, the process was evaluated at laboratory and pilot plant scales.

7.2.1 *Process 1: Production of the Natural Extract.*

The details of Process 1 can be seen in Figure 7.3.

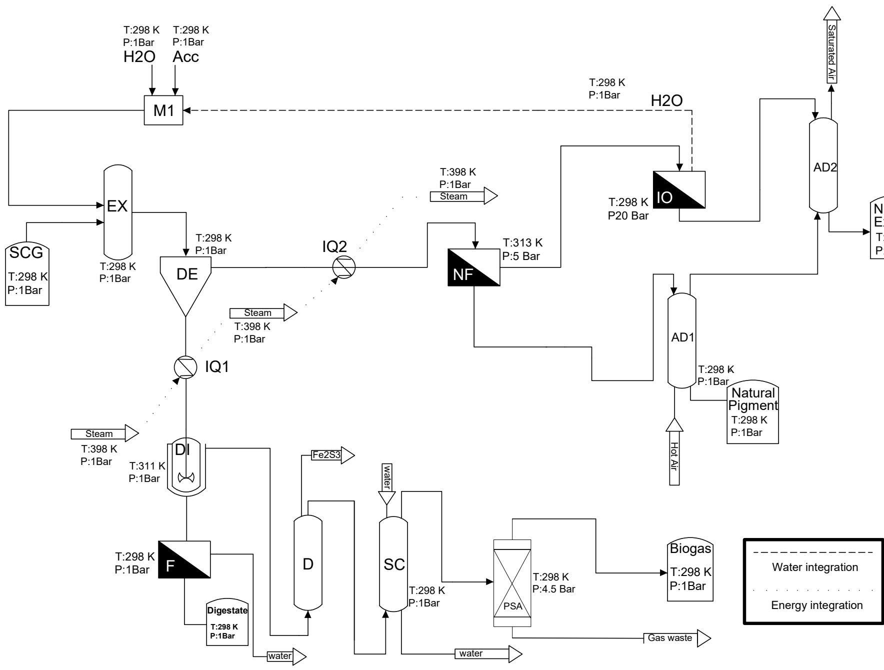

Figure 7.3: Flowsheet diagram of Process 1: Production of Natural Extract from SCG. M represents the mixer.

Among all the products considered in this work, the natural extracts of the spent coffee grounds are the ones with the highest added value. Besides, some additional information is required. It is assumed that the raw material has a humidity percentage of 60% (Brazinha et al., 2015). The mass ratio of the extraction medium (water and a solution of 3 g/L acid citric) with respect to the SCG is 4 (Brazinha et al., 2015), that is to say, 3.988 kg of water and 0.012 kg of acid citric per kg of SCG.

After the extraction process (EX), the solids are distributed between the decanted (precipitated solids) and clarified phase (soluble solids), in the decanter (DE). The mass ratio between the clarified phase and the SCG fed to Process 1 is 3.2 (Brazinha et al., 2015). Therefore, the mass flows of the clarified phase (F_{CLA}) and the decanted phase (F_{DEC}) are calculated from the amount of SCG fed to Process 1 (F_{SCG}) by Eqs. (7.1) and (7.2).

$$F_{CLA} = 3.2 \cdot F_{SCG} \tag{7.1}$$

$$F_{DEC} = 1.8 \cdot F_{SCG} \tag{7.2}$$

In addition, the volume of the clarified phase is also reported (Brazinha et al., 2015), so its density can be calculated (ρ_{CLA}= 1.01 kg/dm^3). This information allows obtaining the composition of soluble solids, water, and citric acid of the clarified stream since the amount of precipitated solids (F_{DECps}) can be estimated using the consideration explained in Section 7.2.2 and the SCG composition (F_{RMts}) (see Table 7.1) is known (Brazinha et al., 2015). The mass balance to the species in the decanted phase, water, precipitated solids, and citric acid is shown by Eq.(7.3). Besides, the concentration of citric acid is 3 g/L (Brazinha et al., 2015) with respect to the amount of water in each phase (Eqs.(7.4) and (7.7)).

$$F_{DEC_{H_2O}} + F_{DEC_{Ac}} + F_{DEC_{ps}} = F_{DEC} \tag{7.3}$$

$$F_{DEC_{Ac}} = 0.003 \cdot F_{DEC_{H_2O}} \tag{7.4}$$

In the case of the clarified phase, the mass flows are given by Eqs.(7.5) and (7.6):

$$F_{CLA_{ss}} = F_{RM_{TS}} - F_{DEC_{ps}} \tag{7.5}$$

$$F_{CLA_{H_2O}} + F_{CLA_{Ac}} + F_{CLA_{ss}} = F_{CLA} \tag{7.6}$$

$$F_{CLA_{Ac}} = 0.003 \cdot F_{CLA_{H_2O}} \tag{7.7}$$

Thus, if the density of the clarified phase is known, the average density of the soluble solids ($\rho_s s$) can be calculated. This is shown in Eq.(7.8).

$$F_{CLA} \cdot \rho_{CLA} = F_{CLA_{H_2O}} \cdot \rho_{H_2O} + F_{CLA_{Ac}} \cdot \rho_{Ac} + F_{CLA_{ss}} \cdot \rho_{ss} \tag{7.8}$$

The density of the soluble solids is later used in the rest of the mass balances. This density determines the distribution of the amount of water between the different phases in the nanofiltration process, but the amount of solids in each phase is known (Brazinha et al., 2015). There is a large amount of water in both phases. Therefore, the error in the approximation is negligible. Precipitated solids (F_{DECps}) are the first type of waste generated in the processing of SCG and are treated by Process A1. The steam to heat-up the stream fed to the nanofiltration process (NF) is generated within the plant by an auxiliary process that uses a fraction of the SCG. This heating is performed in a heat exchanger (IQ2), and the energy balance is presented in Eq.(7.9):

$$\sum_i F_{CLA_i} \cdot cp_i \cdot (40^{o}C - 25^{o}C) = (F_{steam_{in}} - F_{steam_{out}}) \cdot \lambda_{H2O} \tag{7.9}$$

Where cp_i is the heat capacity of each compound of the clarified stream and λ_{H_2O} is the latent heat of the water. In this case, the heat capacity of the liquid water is used since this is the main compound of the stream.

In the nanofiltration process, low molecular weight soluble solids (i.e., caffeine) are separated from high molecular weight solids (i.e., tannins) to adjust the antioxidant properties of the final product so that the product can be sold as a natural coffee extract (Brazinha et al., 2015). Besides, citric acid is retained in this stage (Brazinha et al., 2015).

The amount of solids that go through the nanofiltration process, $F_{PERsslm}$, is determined using the information on the final product presented by the literature (Brazinha et al., 2015). The production yield with respect to the SCG feed and the humidity of the final product (natural extract) are 0.8% and 5.9%, respectively. Therefore, the amount of solids in the natural extract can be calculated as described below. Between the natural extract and the nanofiltration process, there is only reverse osmosis (IO) and a drying process (in both processes, only the water is removed (Brazinha et al., 2015)). Therefore, the amount of solids in the natural extract is the same as in the permeate of the nanofiltration process. The retained solids, $FREN_{sshm}$, can be calculated as the difference between the total solids before the process of nanofiltration, F_{CLAss}, and the solids in the permeate stream ($F_{PERsslm}$)(Eq.(7.10)). The solids retained ($F_{RENsshm}$) are the second type of waste generated in Process 1 and are treated at Process A2. The volume of the retentate is given by the concentration factor, C_{FNF}, with a value of 7.5 in the literature (Brazinha et al., 2015), (Eq. (7.11)), and the mass balance of the compounds of the retentate can be calculated by Eqs.(7.12)-(7.14).

$$F_{REN_{sshm}} = F_{CLA_{ss}} - F_{PER_{sslm}} \tag{7.10}$$

$$V_{REN} = \frac{V_{CLA}}{CF_{NF}} \rightarrow V_{REN} = \frac{F_{REN}}{\rho_{REN}} \rightarrow F_{REN} = V_{REN} \cdot \rho_{REN} \tag{7.11}$$

$$F_{REN_{H_2O}} + F_{REN_{Ac}} + F_{REN_{sshm}} = F_{REN} \tag{7.12}$$

$$F_{REN_{H_20}} \cdot \rho_{H_2O} + F_{REN_{AC}} \cdot \rho_{Ac} + F_{REN_{sshm}} \rho_{ss} = F_{REN} \cdot p_{REN} \tag{7.13}$$

$$F_{REN_{Ac}} = F_{CLA_{AC}} \tag{7.14}$$

In the case of the permeate, the amount of each compound 'i' can be calculated as the difference between the amount of the compounds of the retentate and the clarified phase of the decanter (Eq.(7.15)).

$$F_{PER_i} = F_{CLA_i} - F_{REN_i} \tag{7.15}$$

The high molecular weight solids are treated in Process A2, where they are dehydrated in a drying process down to 10% water, while the low molecular weight solids are dehydrated in a reverse osmosis process and dried to reduce the amount of water down to 5.9%, using a hot air dryer (AD) fed with a stream of flue gas generated in an auxiliary process. The concentration factor (CF$_{OI}$) in the case of the reverse osmosis process is 30 (Brazinha et al., 2015) (Eq.(7.16)). In this case, only water is removed (Brazinha et al., 2015) (Eq.(7.17)) exiting as permeate stream (F$_{OIP}$) in the reverse osmosis process. Eqs. (7.18)-(7.20) are used to evaluate the mass balances between the permeate stream and the rejected stream (F$_{OIR}$) and their components.

$$V_{OIR} = \frac{V_{PER}}{CF_{OI}} \rightarrow V_{OIR} = \frac{F_{OIR}}{\rho_{OIR}} \rightarrow F_{OIR} = V_{OIR} \cdot \rho_{OIR} \tag{7.16}$$

$$F_{OIP} = F_{OIP_{H_2O}} \tag{7.17}$$

$$F_{PER} = F_{OIP} + F_{OIR} \tag{7.18}$$

$$F_{OIR} = F_{OIR_{H_2O}} + F_{OIR_{sshm}} \tag{7.19}$$

$$F_{OIR_{H_20}} \cdot \rho_{H_2O} + F_{OIR_{sshm}} \cdot \rho_{ss} = F_{OIR} \cdot p_{OIR} \tag{7.20}$$

In the drying processes, only water is exchanged between the streams. In the case of the drying process of the natural pigment (AD1), the mass balances are shown by Eqs.(7.21)-(7.23). Eq. (7.24)-(7.26) are used to model the drying process of the natural extract (AD2).

$$F_{REN} + F_{FGIAD1} = F_{NP} + F_{FGOAD1} \tag{7.21}$$

$$F_{REN_{H2O}} - F_{NP_{H2O}} = F_{FGOAD1_{H2O}} - F_{FGIAD1_{H2O}} \tag{7.22}$$

$$F_{NP_{H2O}} = 0.1 \cdot F_{NP} \tag{7.23}$$

$$F_{OIR} + F_{FGIAD2} = F_{NE} + F_{FGOAD2} \tag{7.24}$$

$$F_{OIR_{H2O}} - F_{NE_{H2O}} = F_{FGOAD2_{H2O}} - F_{FGIAD2_{H2O}} \tag{7.25}$$

$$F_{NE_{H2O}} = 0.059 \cdot F_{NE} \tag{7.26}$$

Based on the mass balances presented and described above, Process 1 is modeled within the superstructure.

7.2.2 *Process 2 and Process A1: Production of Biogas and Digestate.*

The same technology (anaerobic digestion) is used in both processes to produce biogas and digestate. The difference is the raw material they use. In Process 2, SCG is used as raw material, while Process A1 uses the precipitated solids from the decanter of Process 1 (see Figure 7.1). The process flow diagram of both processes can be seen in Figure 7.4.

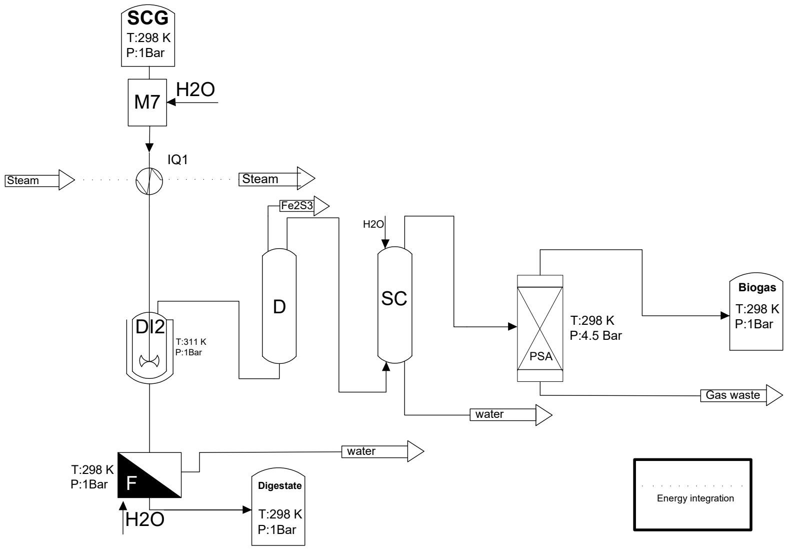

Figure 7.4: Flowsheet diagram of Processes A1 and 2: Production of Biogas and Digestate.

The composition for the SCG is taken from the literature (Vítěz et al., 2016), but in the case of precipitated solids, their composition must be estimated, since the composition is not indicated in the experimental study (Brazinha et al., 2015). The initial composition of the SCG and the following considerations are used to estimate it.

- The nitrogen present in SCG is divided into proteins and nonprotein nitrogen (NPN). The proportion of the nitrogen in the SCG is 54.34% in the form of protein and 45.66% in the form of NPN (Sikka et al., 1985). Proteins are insoluble because, after the production of the soluble coffee, the protein suffers a denaturation and association with cell wall arabinogalactans.(Campos-Vega et al., 2015) In addition, 62.57% of the NPN is soluble in water (Sikka et al., 1985). Considering that it is distributed in the same way in the water of the clarified phase and the water of the precipitated phase and that the ratio of the amount of water in the clarified phase with respect to that in the precipitated phase is 2.11 (Brazinha et al., 2015), 32.25% of the soluble NPN is retained by the precipitate.
- Most carbohydrates are formed by cellulose, hemi-cellulose, and lignin (Campos-Vega et al., 2015). These compounds are insoluble in water (Pedras et al., 2019) under the process conditions (1 bar and 25°C), so it is considered that the carbohydrates after the decantation process are the same that the carbohydrates in the raw material.

Thus, the composition of the precipitated solids is shown in Table 7.1.

Table 7.1: Amount of the precipitated solids (31.01kg)

Compound	Amount (kg)
Ash	0.484
Lignin	6.132
Protein	2.667
Lipids	5.600
Carbohydrates	14.838
NPN (soluble)	0.452
NPN (insoluble)	0.839

This composition is used to model the anaerobic digestion of the precipitated solids. The reactor yield is obtained by running a detailed kinetic model of the process (Taifouris & Martín, 2018) . In this model, an empirical formula for the proteins, carbohydrates, and lipids is considered (Taifouris & Martín, 2018) to calculate the mass and energy balances.

The kinetics is modeled based on the following considerations (Taifouris & Martín, 2018).

- The kinetics follows a first-order reaction where the limiting phase is hydrolysis.
- The reaction is carried out in a stirred thermostated batch reactor to keep the temperature constant.

The kinetic constants are obtained by fitting the kinetic model to the experimental data (Vítěz et al., 2016). Therefore, the stream has to be heated up to 311 K (IQ1 in Process 2 (see Figure 7.4) and in Process A1 (see Figure 7.3)). The rest of the considerations and the kinetic model can be seen in the previous work (Taifouris & Martín, 2018).

This model is solved in Matlab, and a surrogate in the form of an input-output model is formulated to be integrated into the optimization model using the yield toward CH_4,CO_2,SH_2, and NH3 and raw material consumed. The residence time must be equal to or less than 21 days since the reference study (Vítěz et al., 2016) only has data until that day to avoid extrapolation errors. Therefore, only up to 80% of the raw material is used. The profile of the concentration of the components involved in the reaction in the time can be seen in Figure 7.5.

Thus, the reaction yield and its kinetics, the Dalton's and Raoult's principles, as well as Antoine's equation, are used to determine the gas compo-

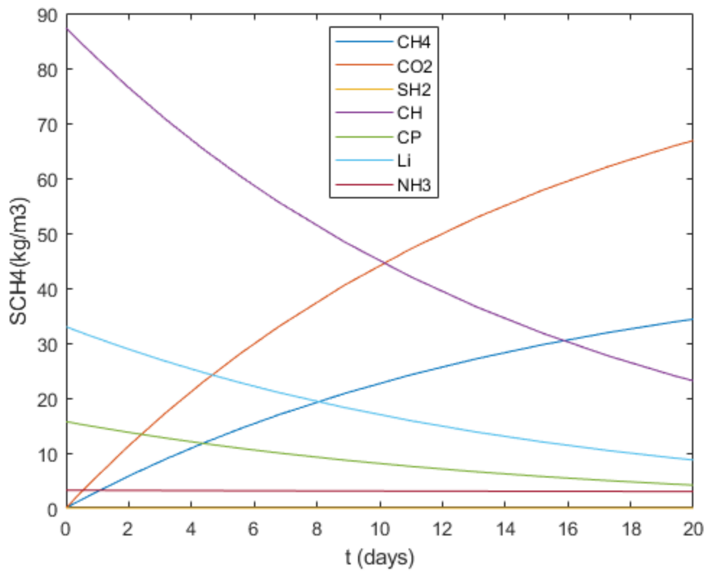

Figure 7.5: Profile of the chemical species along the anaerobic digestion.

sition exiting the digester (DI). This approach was chosen, considering a large amount of liquid-phase water compared to other gases (Sinnot, 2005). The ratio between the molar fraction in the liquid phase and the gas phase is given by Eq.(7.27).

$$\frac{1}{10^{A-\frac{B}{C+T}} \cdot x_i} = y_i \tag{7.27}$$

A bed of Fe_2O_3 (D) is used to remove the H_2S (Martín-Hernández et al., 2020), a scrubber (SC) is used to reduce the amount of ammonia down to 5%,(Taifouris & Martín, 2018) and a pressure swing adsorption (PSA) is used to remove the rest of the ammonia, the water, and 95% of the CO2 of the biogas (Martín-Hernández et al., 2020). A granular filter (F) is installed to dry the digestate.(Taifouris & Martín, 2018) The water consumption of the scrubber is 24.55 m^3 per ton of biogas, while, in the case of the filter, it is 0.01 m^3 per ton of digestate for the cleaning cycle (López et al., 2015).

7.2.3 *Process A2: Production of Natural Pigment*

The flowsheet of process A2 can be seen in Figure 7.6.

This process is fed by the solids retained in the nanofiltration process. These solids are concentrated in tannins. The size of these particles is larger than the ones containing caffeine and can be retained in the nanofiltration

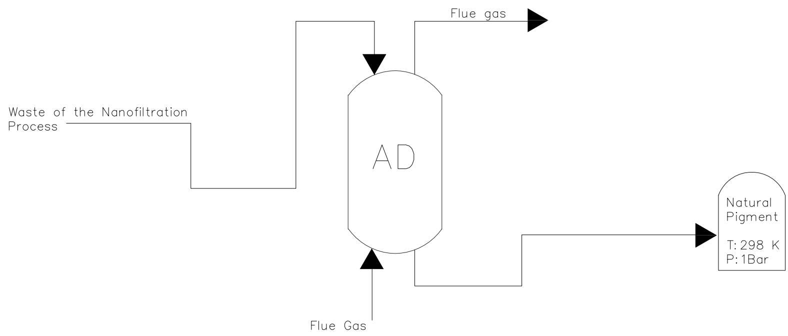

Figure 7.6: Flowsheet diagram of Process A2: Production of Pigment.

process (Brazinha et al., 2015). Since SCG tannins can be used to dye different textiles with brown color(Koh & Hong, 2019), this product can be sold as a natural pigment. The concentration of tannins in these solids was not provided in the experimental study, but the performance to dye a textile sample can be related to the total amount of phenolic components in the solution. The amount of phenolic component needed to correctly dye a gram of textile material is 0.012 g/g textile sample (Koh & Hong, 2019).

The natural pigment is also composed of nonphenolic compounds and a percentage of water. Therefore, the actual ratio is 0.78 g Natural Pigment/g textile. This data will be particularly important to estimate the sale price of this product. The ratio between the phenolic components after the extraction process and the dry spent coffee grounds was experimentally determined (3.31 kg phenolic solids per ton of dried SCG)(Brazinha et al., 2015) and is shown by Eq.(7.28). Furthermore, the yield to natural extract production and the amount of phenolic components in the final product are known (Brazinha et al., 2015). Therefore, the amount of phenolic compounds can be calculated with the amount of raw material (Eq (7.29)). From these two values, the phenolic (Eq.(7.30)) and nonphenolic components (Eq.(7.31)) of the retained solids in the nanofiltration stage can be calculated.

$$F_{CLA_{ssF}} = \left(\frac{3.31}{1000}\right) \cdot (0.4) \cdot F_{RM} \tag{7.28}$$

$$F_{NE_{sshmF}} = 0.02 \cdot 0.008 \cdot F_{RM} \tag{7.29}$$

$$F_{REN_{sshmF}} = F_{CLA_{ssF}} - F_{NE_{sshmF}} \tag{7.30}$$

$$F_{REN_{sshmNF}} = F_{REN_{sshm}} - F_{REN_{sshmF}} \tag{7.31}$$

The nonphenolic components do not affect the dyeing process (Koh & Hong, 2019). The pigment is dried with hot air up to 10% in water to be stored. The hot air is generated by an auxiliary process within the facility.

7.2.4 *Process 3: Production of Power.*

In this case, waste is stored for 3 days, reducing the amount of water from 60% to 10% (Kang et al., 2017). With this final amount of water, the heat of combustion of the SCG is 18.8 MJ/kg (Kang et al., 2017). SCG is considered as a solid fuel (like coal) that can have a yield of 40% to power (integrated gasification combined cycle, IGCC) (Gonzalez, 2009). With this information and the price of the electricity, it is possible to estimate the income obtained from the sale of the produced power from the combustion of the spent coffee grounds, and the operation cost can be estimated using the energy produced (IRENA, 2017). A simplified flowsheet diagram of integrated gasification and the combined cycle can be seen in Figure 7.7.

7.2.5 *Auxiliary Process: Production of Hot Air and Steam*

It is necessary to produce hot air to carry out Process 1 and Process A2 since it is necessary to dry the natural extract and the natural pigment. A fraction of the SCG is sent to a boiler to produce steam and flue gas. To compute it, an energy balance is formulated. The composition of the flue gas is determined by stoichiometry (Roman et al., 2011). The stoichiometry is shown in Eq.(7.32):

$$\begin{aligned} &C_zH_yO_x + r\left(z+\phi-\frac{x}{2}\right)O_2 + r\left(\frac{79}{21}\right)\left(Z+\phi-\frac{x}{2}\right)N_2 \rightarrow \\ &zCO_2 + 2\phi H_2O + r\left(\frac{79}{21}\right)\left(z+\phi-\frac{x}{2}\right)N_2 + (r-1)\left(z+\phi-\frac{x}{2}\right)O_2 \end{aligned} \tag{7.32}$$

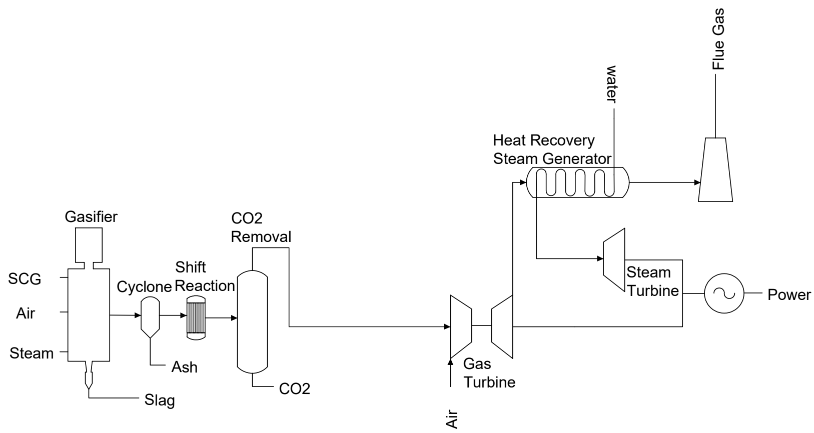

Figure 7.7: Process flow diagram 3.

Where z, y, and x can be obtained from the elemental composition of the spent coffee ground (Silva et al., 1998) and r is the excess air. To achieve the best combustion yield, the excess air should be 1.7 (Silva et al., 1998). However, the air has humidity, and therefore, this equation has to be modified; 15% of the relative humidity and a temperature of 25 °C are considered. The final equation becomes Eq.(7.33):

$$\begin{gathered}C_{0.3433}H_{0.51}O_{0.1335} + 0.69O_2 + 2.584N_2 + 3.372H_2O \rightarrow \\ 0.3433CO_2 + 3.6269H_2O + 2.584N_2 + 0.283O_2\end{gathered} \tag{7.33}$$

It is necessary to compute the fraction of energy to produce steam, which was used to obtain hot flue gas so that the energy balance holds; 60% of the energy of the combustion is used to produce the required heating steam, 30% to heat the flue gas, and 10% of the energy is lost (Silva et al., 1998). With this information, it is possible to formulate the mass and energy balances. The heat of combustion (HC) of the SCG is 18.8MJ/kg (Kang et al., 2017). The energy balance applied to the combustion gases is shown by Eq.(7.34):

$$\eta_{air} \cdot F_{SCG \rightarrow AUX} \cdot HC = \sum_i F_i \cdot cp_i \cdot (T_{out} - T_{in}) \tag{7.34}$$

Where η_{air} is the fraction of heat absorbed by the air, 0.3, $F_{SCG \rightarrow AUX}$ is the mass flow of burned raw material, and HC is the heat of combustion.

F_i is the mass of each component of the flue gas, cp_i is the heat capacity, T_{in} is the air inlet temperature, and T_{out} is the temperature of the flue gas. As the maximum amount of water that the air can remove is a function of its temperature and the amount of air, mass and energy balances of the processes of combustion and drying must be solved simultaneously.

No change in temperature is considered in the streams that are dried to avoid damaging the product. The heat supplied by flue gas must be equal to the heat required to dry the natural pigment down to 10% water and the natural extract down to 5.9%. This energy balance is given by Eq.(7.35):

$$\sum_i F_i \cdot cp_i \cdot \left(T_{out_{FG}} - T_{in_{FG}}\right) = \lambda_{H2O} \cdot \left(F_{H2O_{IN}} - F_{H2O_{OUT}}\right) \tag{7.35}$$

where T_{in} is the inlet temperature of the flue gas into the drying process, T_{out} is the outlet temperature, λ_{H2O} is the latent heat of water, F_{H_2Oin} is the mass flow of water of the stream that goes into the dryer, and F_{H_2Oout} is the mass flow of water of the stream that comes out. The evaporated water is removed by the flue gas, so its humidity increases with each of the two drying stages at Process 1 and Process A2. The relationship between absolute air humidity and partial pressure is indicated by Eq.(7.36).

$$AH = 0.625 \cdot \frac{Pa}{P - Pa} \tag{7.36}$$

The relative humidity must be lower than one in the pigment drying process. Since this flue gas is generated through the combustion of SCG, to reduce the losses of raw material, the target is to minimize its production. Therefore, the relative humidity of the flue gas from the last drying process is fixed to 1.

AH is the absolute humidity (kg water/kg dry air), Pa is the partial pressure of the water, and P is the total pressure, 1 atm. The saturation pressure is calculated using Antoine's equation.

In addition to hot air production, steam is also produced. This steam is used to heat the streams before anaerobic digestion and the stream before the nanofiltration stage. The amount of steam generated is given by Eq.(7.37):

$$\eta_{H2O} \cdot F_{SCG \to AUX} \cdot HC = F_{H2O} \cdot cp_{H2O} \cdot (120^{o}C - 25^{o}C) + \lambda_{H2O} \cdot F_{H2O} \tag{7.37}$$

where η_{H2O} is the percentage of heat absorbed by the water,0.6, and F_{H2O} is the mass flow of steam generated. Note that $F_{SCG \to AUX}$ is the same variable as in Eq.(7.34). Since the amount of steam generated is much larger than the one necessary as a utility in the processes of the superstructure, the rest of the steam can be used in the extraction process of instant coffee production. In the extraction process, the relationship between the steam and the solid total of the product is 28, according to a patent (Pedersen et al., 2014) . Besides, 75 % (Silva et al., 1998) of the necessary energy to produce instant coffee is used in the extraction process. Therefore, it is possible to estimate the steam required by the production of soluble coffee and to supply a part of that energy with the steam of the auxiliary process. As a result, the circular economy and the principle of self-sufficiency are favored.

7.2.6 *Process Using Dried Raw Material*

The most studied process that uses dried SCG is the biodiesel production process, but the raw material has 60% of water; it is necessary to remove that water before feeding the process. For this reason, it is very likely that this type of process is not economically feasible. Therefore, a preliminary study is carried out to determine the maximum income and energy that can be obtained from that biodiesel. The results of the study are that the energy balance is negative, 4698 kcal per 100 kgSCG, due to the yield to produce the biodiesel and the difference between the heat combustion of the SCG and Biodiesel. A quick economic evaluation also shows nonprofitable production, 0.9€ per ton of Biodiesel. Both studies are reported in the Supporting Information.

7.2.7 *Solution Procedure*

7.2.7.1 *Process Design*

The superstructure is solved using a simplified profit as an objective function. The amount of SCG that is sent to each process is a variable of the optimization model and will depend on the operating costs and incomes from the sale of the products generated in each process. The objective function is given by Eq.(7.38) including the income from products and the operating cost and energy:

$$\begin{aligned} \mathrm{Pr}\,ofit = {} & \sum_p \mathrm{PriceProduct_p} \cdot F_p - \sum_i \mathrm{PriceRawMaterial}_i \cdot F_i \\ & - \mathrm{CW} - \mathrm{CE} - \mathrm{C_{PowerPlant}} \cdot HC \cdot F_{SCG \rightarrow P3} \end{aligned} \tag{7.38}$$

where F_i and F_p are the mass flow of the raw material and products, respectively. $F_{SCG \rightarrow P3}$ is the amount of spent coffee grounds that is sent to Process 3. CE and CW are the production cost of the electrical and thermal energy, respectively. $C_{powerplant}$ is the operating cost of the power plant.

Raw Material Cost. We consider the cost of the spent coffee grounds, citric acid, and water. The prices can be seen in Table 7.2.

Table 7.2: Price of the raw material

Raw material	Cost(€/t)
Spent Coffee Ground (Brazinha et al., 2015)	50
Citric Acid (ECHEMI, 2020)	530
Water (Trata Brasil: Saneamento é saúde, 2020)	0.78

Cost of Energy. Both electrical and thermal energy are considered. On the one hand, most of the electrical energy used in the plant is consumed by the pumps necessary to feed the processes of reverse osmosis (20 bar) and nanofiltration (5 bar). For the calculation of this type of energy, the consumption of power by a pump is computed using Eq.(7.39) for nanofiltration and Eq.(7.40) for reverse osmosis:

$$Pw_{NF} = n_{NF} \cdot p_{H2O} \cdot g \cdot V_{CLA} \cdot h_{NF} \tag{7.39}$$

$$Pw_{IO} = n_{IO} \cdot p_{H2O} \cdot g \cdot V_{PER} \cdot h_{IO} \tag{7.40}$$

where η_{NF} and η_{IO} are the eficiencies of the pump (0.55 for the nanofiltration process and 0.47 for the reverse osmosis process (Sinnot, 2005)). h_{NF} and h_{IO} are the hydraulic heights that are computed performing an energy balance, the Bernoulli equation, to the pump resulting in values of 41.37 and 165.43 m for nanofiltration and reverse osmosis process, respectively. Considering that the electrical energy is produced in the plant using raw material, the cost of electricity will be equal to the cost of the raw material used to produce that energy. Taking into account the considerations indicated in Section 7.2.4 and the cost of the raw material, the cost of the energy consumed by reverse osmosis and nanofiltration processes can be estimated by Eq.(7.41), where C_{RM} is the cost of the spent coffee grounds.

$$CW = (Pw_{Nano} + Pw_{OI}) \cdot \tau \cdot HC \cdot 0.4 \cdot F_{RM} \cdot C_{RM} \tag{7.41}$$

On the other hand, most of the thermal energy used in the plant is used in the drying processes for the production of the natural extract (Process 1) and the natural pigment (Process A2). The value corresponds to the energy required to evaporate the water accompanying both products. Its cost is computed as the amount of SCG needed to produce the energy. In this way, the thermal energy cost to dry the natural pigment and the natural extract is calculated by Eq. (7.42) and Eq. (7.43). The total cost is given by Eq.(7.44):

$$CE_{NE} = \frac{(\mathrm{F}_{\mathrm{NE}_{\mathrm{H2O}_{\mathrm{in}}}} \text{-} \mathrm{F}_{\mathrm{NE}_{\mathrm{H2O}_{\mathrm{out}}}})}{(\mathrm{F}_{\mathrm{NE}_{\mathrm{H2O}_{\mathrm{in}}}} \text{-} \mathrm{F}_{\mathrm{NE}_{\mathrm{H2O}_{\mathrm{out}}}}) + (F_{NP_{\mathrm{H2O}_{\mathrm{in}}}} \text{-} \mathrm{F}_{\mathrm{NP}_{\mathrm{H2O}_{\mathrm{out}}}})} \cdot \mathrm{F}_{\mathrm{SCG} \rightarrow \mathrm{AUX}} \cdot C_{RM} \tag{7.42}$$

$$CE_{NP} = \frac{(\mathrm{F}_{\mathrm{NP}_{\mathrm{H2O}_{\mathrm{in}}}} \text{-} \mathrm{F}_{\mathrm{NP}_{\mathrm{H2O}_{\mathrm{out}}}})}{(\mathrm{F}_{\mathrm{NE}_{\mathrm{H2O}_{\mathrm{in}}}} \text{-} \mathrm{F}_{\mathrm{NE}_{\mathrm{H2O}_{\mathrm{out}}}}) + (F_{NP_{\mathrm{H2O}_{\mathrm{in}}}} \text{-} \mathrm{F}_{\mathrm{NP}_{\mathrm{H2O}_{\mathrm{out}}}})} \cdot \mathrm{F}_{\mathrm{SCG} \rightarrow \mathrm{AUX}} \cdot C_{RM} \tag{7.43}$$

$$CE = CE_{NE} + CE_{NP} \tag{7.44}$$

Operating Cost of the Power Plant. It is possible to estimate the operating costs of a power plant from biomass using data from the literature (IRENA, 2017). The operational costs are given by Eq.(7.45).

$$\mathrm{C} = 0.06€/kW \tag{7.45}$$

Income from the Products. The income of the natural extracts, natural pigment, biogas, digestate, and power are considered. In the case of natural extracts, the same price in Brazinha et al., 2015 (70€/kg natural extracts) is used. It is considered that the biogas is used to produce power; therefore, its price is estimated using the price of the power (0.1021€/kWh) (Organismo Supervisor de la Inversion en Energía y Minería, 2018), the yield to produce power from a gas fuel (40% (Asís et al., 2005)), and heat of combustion of 5500 kcal/m^3 (IRENA), 2015). The income of the digestate is estimated using the price of fertilizer (182.16€/t (Brasil, 2020)). Following the classification criteria of natural pigments used by a company specialized in the sale of this type of product (Maiwa, 2020), the main factor used to estimate the price is the weight of fiber (WOF) (Maiwa, 2019). WOF is calculated following Eq. (7.46):

$$WOF = \frac{Weight\ Natural\ Pigment}{Weight\ Textile\ Sample} \cdot 100 \tag{7.46}$$

In the case of the natural pigment of this work, the ratio is 0.78 g natural pigment/g textile, and therefore, the WOF is 78%. The price of this product can be estimated using a similar natural pigment (Maiwa, 2020), whose sale price is 28€/kg. Finally, the price of the power is 0.1021 €/kWh (Organismo Supervisor de la Inversion en Energía y Minería, 2018), and the yields indicated in Section 7.2.4 are used to estimate the income of the power produced using the SCG that is sent to Process 3. The optimization formulation is subjected to the models described in Sections 7.2.1-7.2.5.

Model Statistics and Solution. The model is a nonlineal programing (NLP) model and consists of 610 equations and 1615 variables. KNITRO and CONOPT are used to find an initial feasible solution, and BARON is used to find a global optimum for the problem (gap of 0.2%). The use of binaries was avoided so as not to formulate mixed-integer nonlinear programming (MINLP). Continuous variables (flows of raw materials sent to different processes) were used to decide whether the process is used or not.

7.2.7.2 *Investment and Production Costs of the Factory.*

The investment and production costs associated with the use of SCG as raw material are estimated using the factorial method (Sinnott, 2005) . The investment cost is based on the equipment cost that is computed unit by unit from their size and using cost correlations appropriated to each unit type. The production costs involve raw materials, maintenance, labor, among others. Further considerations and calculations are included in the Supporting Information.

7.3 RESULTS

One of the main problems in the development of biorefineries aimed at treating this type of waste is the decentralization of its production. Approximately, 50% of the SCG is generated in coffee shops and restaurants and by private consumption (Cruz et al., 2012), and its collection is challenging because individual production is very low. The high content of water and organic matter makes its transport and storage also a difficult task, due to the degradation processes. The other 50% is generated in the processes of soluble coffee production. In addition, the performance also depends on the quantity and quality of the raw material sent to the biorefinery, so it is important to ensure that the raw material for the biorefinery is homogeneous in both quality and quantity. Therefore, it is assumed that the processing of SCG will be an additional section to the soluble coffee production process. In this way, the initial conditions of the waste will not vary significantly. The standard size of a soluble coffee production plant varies between 16500 and 23000 tons per year (Murthy & Naidu, 2012). Therefore, the production of 40000 t/year of SCG (2 kg of SCG are produced by 1 kg of soluble coffee produced (Rajesh et al., 2020)) is used to test the methodology explained in Section 7.2. The results are divided into two sections. The results corresponding to the mass and energy balances of the process are selected as optimal and the economic evaluation of each of the processes.

7.3.1 *Mass and energy balances*

All of the processes previously described are considered simultaneously in the same optimization model. The amount of SCG sent to each process is a variable of the problem. The results show that 58.94% of the raw material is sent to Process 1, while 41.06% is used for the production of utilities for the process. This amount is the minimum necessary to generate hot air for the drying processes. The yield of natural extract production is 0.494%, while that of natural pigment is 4.88% (with respect to the initial SCG). The yield to natural extract is slightly lower than the one indicated in the literature (Rico & Sánche, 2005) (0.8%). Nevertheless, this is due to the fact that part of the SCG is being used to produce energy, and the yield is calculated considering the entire amount of SCG (40000t). The biogas and digestate production yields are 3.13% and 10.66%, respectively. Table 7.3 shows a summary of the main results.

It can be seen that when the added value of a product is larger, its yield is lower. The product that shows the best trade-off is the natural pigment since its price is high and the yield is not particularly low. In the opposite case, the biogas has a low yield and low price.

The water reused within the process allows a reduction in the consumption of fresh water of 32.6%. The output water from the digestate filtration process could have been used in the scrubber (see Figure 7.1); however, the dissolved ammonia did not allow it. By using a fraction of SCG as fuel, the use of nonrenewable electrical energy is avoided. In addition, it is observed that the amount of steam generated in the plant is much larger than what is necessary (only 6.6% is used by the new line of the factory). This is because the consumption of the boiler is adjusted to produce the flue gas necessary for the drying processes, while the steam generated is

Table 7.3: Mass Balances of the best process

Products	Amount (t/year)
Dried natural extract	198
Dried natural Pigment	1951
Biogas	1255
Digestate	4264
Steam	57287
Raw material	**Amount (t/year)**
Total SCG	40000
SCG for the process 1	23577
SCG for the process 2	0
SCG for the process 3	0
SCG for the auxiliary process	16423
Consumed water (With water integration)	129807
Consumed water (Without water integration)	192592
Citric Acid	324
Steam	4032
Air for the combustion process	346650

considered as a secondary asset (see Eq.7.33). Therefore, it is possible to use this steam to supply the heating utility for the extraction process of the production of instant coffee. The excess of steam produced from the SCG represents 9.5% of the total steam required in the extraction process. Since the extraction process represents 75% of the energy of the entire instant coffee production process, the steam generated in the auxiliary process allows saving 7% of the total energy. As a result of the integration of the use of SCG within a soluble coffee facility, 7925tCO_2/year can be avoided versus the use of natural gas (Junta de Castilla y León, 2020) or 18328tCO_2/year if the steam is generated with coal (IRENA), 2015). The amount of SCG needed to generate all of the steam needed to supply the extraction process for soluble coffee would be 186667t. Therefore, the maximum amount of steam savings that can be achieved, assuming that all of the SCG generated in the soluble coffee production process are sent to the boiler, would be 21.5%.

7.3.2 *Economic Evaluation.*

The income and costs considered by the objective function determine the transformation route that is the most profitable. Once the best process is established, a more detailed economic evaluation is carried out. As indicated in the previous section, most of the available raw material is sent to Process 1, so this is the best process from an economic point of view. Table 7.4 shows the results of income and cost considered in the objective function for Process 1.

Table 7.4: Income and main variable operating costs

Item	(k€/year)
Income of pigment	54637
Income of natural extract	13838
Income of digestate	777
Income of biogas	152
Total income	69403
Cost of raw material	1179
Cost of citric acid	172
Cost of water	101
Cost of heat energy	821
Cost of electric energy	3
Main variable operating costs	2276

On the one hand, the products that generate the largest income from Process 1 are the natural extract and the natural pigment, which represent 19.93% and 78.72% of the total income, respectively. This is because both are highly added-value products, despite the low amount produced. The waste produced in a decanter is used to produce biogas and digestate, even though the income of these products is low, representing 0.22% and 1.12% of the total, respectively. On the other hand, the highest operating cost is associated with the raw material, representing 51.80% of total operational costs, while citric acid represents 7.56%, the water 4.44%, and the energy 36%. This is because the amount of citric acid used is very small, water is a cheap chemical compound, and the energy consumption is not very high. In addition, we reduce the consumption of energy in the drying process through the prefiltering process, and the hot air, steam, and power are produced at the factory.

A complete economic analysis, considering operating costs and fixed capital, is carried out for Process 1, since this process is the most profitable. Table 7.5 shows the results of the detailed economic analysis.

Table 7.5: Results of the complete economic analysis

Total investment(M€)	
PCE	4.05
PPC	9.51
Fixed Capital	13.31
Working Capital	0.66
Total	13.97
Operation Cost(M€/year)	
Variable	
Raw materials	1.35
Miscellaneous	0.06
Utilities	0.10
Power	0.82
Fixed	
Maintenance	0.66
Operating Labour	0.08
Plant overheads	0.04
Laboratory	0.02
Capital Charges	1.33
Insurance	0.13
Total	4.59
Annual profit(M€/year)	64.81

The objective function only considers the major variable contributions, which represent almost 50% of the total operating costs. It is assumed that labor and laboratory costs will be similar in all of the processes considered. In addition, there is a large difference in the profits obtained among the set of processes involved in the superstructure. Therefore the objective function is considered to correctly select the most profitable process.

On the one hand, regarding the investment costs, the highest share corresponds to the cost of the digesters, which represents 48% of the total, because of the high residence time necessary for the conversion of the waste into biogas and digestate. First, the possibility of not treating these wastes was considered to avoid the cost of the digesters, but one of the objectives of this work is to use all of the waste produced in the processes (that can be treated) toward implementing the circular economy concept within the food industry, aiming at zero-waste emissions. Therefore, that cost was considered in the analysis. On the other hand, regarding the operating costs, the highest is the cost of raw material, which represents about 29% of the total costs. Note that the income from the sale of the products allows for the recovery of the investment in the first year of installation. This is because the price used to estimate the income of the products is the final price in a retail establishment. It is expected that the manufacturing price and the final sale price differ considerably; however, this price is considered an industrial secret and is very difficult to estimate. For this reason, in the last part of this section, a sensitivity study is carried out, considering different prices and demands.

7.3.3 *Alternative Solutions*

It is possible to process the SCG following also Processes 2 and 3. While the optimization does not select these alternatives based on poorer economic potential, in this section, the economic performance of Process 1 compared with other processes proposed in this study is presented. The amount sent to each process was set to analyze the maximum benefits that the factory would have if other processes were selected. An economic evaluation of Processes 2 and 3 can be seen in Table 7.6.

Table 7.6: Economic evaluation of the Process 2 and 3

Process 2	
Item	(k€/year)
Income of biogas	267
Income of digestate	1958
Total income	2225
Cost of raw material	2000
Cost of water	162
Operational total cost	2162
Profit of the process 2	61
Process 3	
Item	(k€/year)
Incomes of power	8529
Operational total cost	4795
Cost of raw material	2000
Operational total cost	6795
Profit of the process 3	1734

In the case of Process 2, the operating costs are similar to the income, and therefore, the profit is low. In fact, the profitis almost 29 times lower than the profit of Process 3 and 1140 times lower than the profit of Process 1. In addition, it is necessary to indicate that the amortization costs of the equipment for each process are not being considered when selecting the processes. If this cost is added in the economic evaluation, this process would not be profitable, and it would be necessary to discard it when carrying out a more detailed analysis of each of the processes. However, unlike what happened with biodiesel, which can be determined not to be competitive with a preliminary study, in this case, the difference between incomes and costs is quite small and cannot be discarded in a preliminary study. Finally, Process 3 is economically viable, but its profit is worse than Process 1, 40 times less (IRENA, 2017).

Nevertheless, these processes are clearly less profitable than Process 1, and the profit of this process is subject to great uncertainty for two main reasons. The variability in the prices of high added-value products is especially high since it depends on the type of markets and the countries where they are sold, and their price can vary by orders of magnitude. The products obtained from waste must compete for a market gap or displace those obtained from natural or artificial sources, which are usually of better quality and lower price. For these reasons, a sensitivity study is performed in order to establish the critical values from which Process 3 began to be competitive compared to Process 1, using the flexibility that the superstructure allows. Process 2 is discarded due to its low profit margin. Three prices and three percentages of product sold are established for each product. The demand had to decrease to values lower than 10% to be able to reach the critical values of the optimal process change due to the great difference in profit between Processes 1 and 3. The complete results of the sensitivity study can be found in the Supporting Information. The most important results from this analysis are shown in Table 7.7.

Table 7.7: Summary of the sensitivity analysis

Scenario	Pnp(€/kg)	Pne(€/kg)	Dnp (%)	Dne(%)	Profit(M€/year)	Optimal process selected
1	14	35	3	3	598	3
2	14	50	3	3	687	3
3	14	70	3	3	806	3
12	14	70	6	3	1717	3
35	20	50	3	10	1770	1
79	28	35	10	10	6249	1
80	28	50	10	10	6545	1
81	28	70	10	10	6941	1

In addition to the specific results obtained in the present case study, the flexibility of the superstructure designed in the present work allows for adaptation to the particular market conditions of the place under consideration. Pnp and Pne are the prices of the natural pigment and the natural extract, respectively. Dnp and Dne are the percentages sold of natural pigment and natural extract.

After the analysis, it can be seen that scenarios 1, 2, and 3 show the worst possible combination of the parameters, while scenarios 79, 80, and 81 show the best results for a demand of 10% of the total material manufactured. Scenarios 12 and 35 constitute the critical values from which Process 1 is no longer the most profitable.

7.4 CONCLUSIONS

The analysis of the use of SCG as a resource to produce added-value products and energy has been analyzed from the process perspective within a biorefinery concept. A superstructure has been developed where three different processes are considered to produce five products (natural extract, natural pigment for the textile industry, biogas, digestate, and power).

Mathematical optimization techniques are used to select the best process and the portfolio of products from an economic point of view.

In addition, the integration of energy and water is considered. Due to the decentralized production of the spent coffee grounds and its high water content, it was decided that the process is integrated as an additional production line to the soluble coffee production process, and a fraction of the remaining energy of the recovery process is used to drive the main production process.

After analyzing different alternatives, two processes are economically viable, the production of energy, Process 3, and the production of natural extract and pigment, Process 1. Nevertheless, Process 1 shows a profit 40 times higher than Process 3 due to the high sale price of the natural pigment and of the natural extract, and therefore, this process is chosen for the valorization of the SCG. Between these two products, the income from the sale of natural pigments is 3.9 times higher than the natural extract, which makes natural pigment the most balanced product in terms of price and production capacity. The annual profit using Process 1 is 65 MM€/year, while operating costs are 4.59MM €/year. Regarding investment costs, 13.97 MM€ is necessary to start up the new production line based on Process 1. The digesters are the most expensive equipment (48% of the total equipment cost); nevertheless, they are necessary for the treatment of the waste produced in the decantation process. The treatment of these wastes was maintained to comply with the treatment of all wastes generated since the benefits of the sale of digestate and biogas (0.77 MM€/year and 0.15 MM€/year, respectively) are negligible compared to other products.

The use of SCG to produce biodiesel is discarded due to the need to dry the raw material. Digestate and biogas production using the SCG as raw material (Process 2) is discarded because it has a negative benefit when all operating costs are considered.

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8

EVALUATION OF THE ECONOMIC, ENVIRONMENTAL AND SOCIAL IMPACT OF THE VALORIZATION OF GRAPE POMACE FROM THE WINE INDUSTRY

ABSTRACT

The increase in world population has led to intensive food production systems that are generating increasing amounts of solid waste. In this work, the valorization of the most important waste generated during wine production, grape pomace, is evaluated. Eight processes are proposed to approach different types of valorization (production of energy and value-added products), from an economic, environmental and social points of view. The best process depends on the budget available, the production capacity and the weight of each impact produced by the factory (economic, environmental or social). For small (less than 0.1 kg/s) or very large (greater than 10 kg/s) capacities, the production of high value-added products outperforms the other processes in all three impacts and in profitability. For intermediate capacities, combustion and gasification have a low economic impact and a high environmental impact, anaerobic digestion stands out as having the lowest environmental impact, and tannin production is the best balanced process, with high economic and social impacts. Pyrolysis is the worst process in all three impacts.

keywords: Agricultural residues, Sustainable process design, Energy, Circular Economy, High-valued products

RESUMEN

El aumento de la población mundial ha llevado a sistemas intensivos de producción de alimentos que generan cantidades cada vez mayores de residuos sólidos. En este trabajo, se evalúa la valorización del residuo más importante generado durante la producción de vino, la pulpa de uva. Se proponen ocho procesos para abordar diferentes tipos de valorización (producción de energía y productos de alto valor añadido), desde un punto de vista económico, ambiental y social. El mejor proceso depende del presupuesto disponible, la capacidad de producción y el peso de cada impacto producido por la planta (económico, ambiental o social). Para capacidades pequeñas (menos de 0,1 kg/s) o muy grandes (mayores de 10 kg/s), la producción de productos de alto valor añadido supera a los demás procesos en los tres impactos y en rentabilidad. Para capacidades intermedias, la combustión y gasificación tienen un bajo impacto económico y alto impacto ambiental, la digestión anaerobia destaca por tener el menor impacto ambiental, y la producción de taninos es el proceso mejor equilibrado, con altos impactos económicos y sociales. La pirólisis es el peor proceso en los tres impactos.

Palabras clave: Residuos agroindustriales, desarrollo de procesos sostenibles, energía, economía circular, productos de alto valor añadido.

8.1 INTRODUCTION

The growth of the world population has resulted in the intensification of food production processes, which results in an increment in the amount of organic solid waste produced annually. This situation leads to an increased risk of nutrient pollution as long as they are not treated properly (Minghua et al., 2009). This, together with greater environmental awareness on the part of governments, which has resulted in environmental policies (Commission, 2020), has pushed companies to change their production systems. The design of these new processes takes into account the concepts of circular economy and zero-emission philosophy (European Commission, 2020). One of the largest contributors to solid waste generation in the food industry is wine production (Ahmad et al., 2020), especially in Italy, France, Spain (Europe, 2021), and California (USA) (The national association of american wineries, 2022). During the wine production process, up to 200 kg of solid waste are generated per 750 liters of wine produced. Of this solid waste, 60% consists of a mixture of grape skins and seed, representing the grape stalks, wastewater, and wine lees the rest. This waste is known as grape pomace (Jin et al., 2021). Grape pomace is often deposited in large aeration tanks (Ahmad et al., 2020), which does not only cause a massive loss of value but can also cause nutrient pollution due to its high concentration of organic matter.

There is a wide variety of techno-economic studies that advocate the possibility of obtaining economic and environmental benefits by using this residue as a source of added-value products and energy. Grape pomace is an important source of polyphenols and essential oils, which are antioxidant, antimicrobial, anti-inflammatory and anticarcinogenic, and can be used as food additives or pharmaceuticals (Jin et al., 2021). In addition to these products, chemical, physical and biological processes can be used to produce fertilizers (Achkar et al., 2016), biochar (Ferjani et al., 2019), tannins (Ping et al., 2011) and biofuels such as biodiesel (Bolonio et al., 2019) and bioethanol (Corbin et al., 2015). The composting of grape pomace allows this residue to be used to improve soil properties or as animal feed (Alba et al., 2019; Cortés et al., 2020). Finally, grape pomace can be used to produce power directly through thermal processes such as combustion, gasification, or pyrolysis (Ramos & Ferreira, 2022).

However, these studies usually cover a limited set of processes applied to very specific cases (production capacity or a specific grape pomace composition), which are studied separately. The economies of scale associated with the production capacity of the treatment plant, together with a production yield dependent on the composition of the waste, means that these processes cannot be directly compared. Therefore, it is difficult to select the best option for different production capacities, physicochemical properties of the residues and capital available for investment. On the one hand, it is not possible to evaluate the synergies that may exist between processes, such as secondary waste valorization, energy, and water integration or shared supply chains. On the other hand, many of these studies only focus on the economic dimension, leaving aside the environmental and social impacts of each process. To the best of the authors' knowledge, there is no work that simultaneously analyzes all the types of grape pomace valorization (energy valorization and production of value-added products), evaluating the economic, environmental and social impact of each process, for different production capacities and budgets, under the same framework and estimation methods.

The concept of integrated biorefineries represents the optimal approach to treat organic residues (Ncube et al., 2021) due to the complexity of their compositions. These biorefineries make it possible to obtain a set of added-value products by integrating a series of chemical and physical processes at the same time, in series or parallel lines, whitin a single facility. This reduces the waste generation, by taking advantage of synergies, such as energy and water integration, secondary waste treatment, among others. Besides, the profitability of the process is higher due to the generation of a wider range of products (Jin et al., 2018). Although it has been a widely studied in recent years (Martinez et al., 2016; Ncube et al., 2021), this type of biorefinery requires an investment capital that may be too high for small wineries (Jin et al., 2021). It is therefore very important to analyze both simple and complex processes to address wine industries with different production capacities and available capital.

Therefore, in this work, a framework, which contains 8 different processes of grape pomace valorization, is developed to analyze the more promising technology to optain value from differents points of view (economic, environmental, and social). Between the considered processes, there are two devoted to produce power (combustion and gasification), four to produce fertilizers (anaerobic digestion), biochar (pyrolisis), tannins and essential oils (extraction-filtration system) and a last process to obtain polyphenols (extraction-purification system). Each process is modeled using first principles such as mass and energy balances, thermodynamic equilibrium, empirical correlations and performances (Martin, 2021). This allows determining which is the best process for different capacities, for different budgets and from different points of view (economic, environmental, and social). Furthermore, it analyzes possible combinations of processes to reduce the environmental impact and improve both the economic and social impacts. The paper is structured as follows. Section 8.2 explains how the different processes have been modeled and how the economic, environmental and social evaluation has been carried out. Section 8.3 presents the case study used to evaluate the model designed in the previous section, and shows the results of the analysis. Finally, Section 8.4 presents the most significant conclusions on the results of the research.

8.2 FRAMEWORK DEVELOPMENT

8.2.1 *Estimation of the production and composition of the grape pomace*

Following the work of Rodrigues et al., 2022 , it is estimated that 0.16 kg of grape pomace is produced per liter of wine. Therefore, grape pomace production is estimated from wine production, following public information on winery sales. The estimation of the composition of grape pomace is more complicated because it can change depending on the reference consulted since it is a waste that is strongly dependent on the type of grape and wine production. Therefore, it is essential that the mathematical model takes into account the grape composition in order to estimate the economic, environmental and social impacts of the treatment processes. In order to calibrate the models presented in this section, a particular grape pomace composition estimated from different references, is used and shown in Table F.3 of the supplementary material. In spite of the fact that this study focuses on the valorization of grape pomace, some of the processes, such as anaerobic digestion, gasification or extraction, can be used to treat the rest of the waste generated during winemaking, such as lees and waste water.

8.2.2 *Processes analysis and design*

The processes shown in this Section are modeled following first principles, such as mass and energy balances, thermodynamic equilibria, empirical correlations or yields, based on information from different works used as references. Since there is a model for each process, the optimization framework consists of eight mathematical models. Each model is optimized to maximize profit, although the environmental and social impact are also evaluated, following the procedures described in Section 8.2.3.

The processes are divided into three groups. Combustion and gasification are aimed at producing energy from grape pomace, while the rest of the processes are used to obtain chemical products, which can be classified into valued and high-value products, depending on their market value. On the one hand, anaerobic digestion, pyrolysis and an extraction-filtration system are used to produce fertilizer, biochar, and tannins, which constitute the group of valued products. On the other hand, an extraction-purification system is used to obtain polyphenols and essencials oils, the products considered as high-value product in this work.

8.2.2.1 *Energy production*

There are three processes that use grape pomace to obtain energy: combustion, gasification and pyrolysis. However, in this section, only the first two are considered for obtaining energy since pyrolysis can be used to produce biochar, which is considered an added-value product. The flowsheets for combustion and gasification can be seen in Figure 8.1.

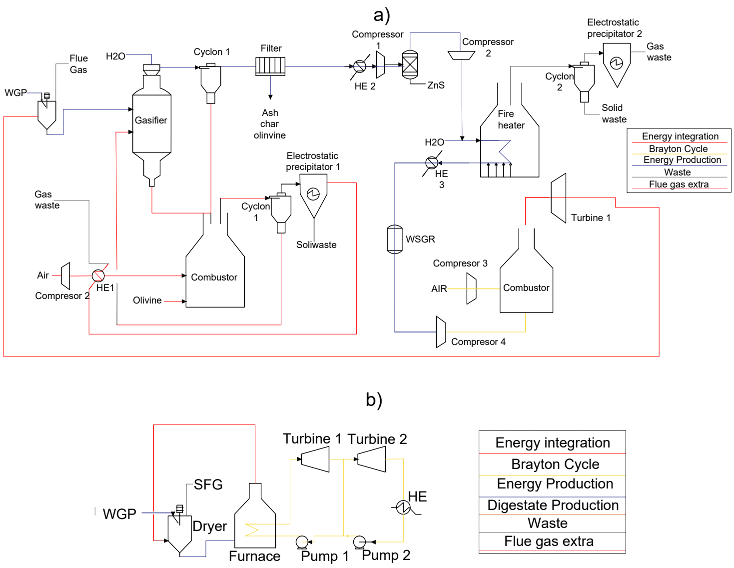


Figure 8.1: Flowcharts of the process which produce power (a: Gasification and b: Combustion)

First, it is necessary to dry the raw material to 10 % moisture content for both processes. Although natural drying (storing the raw material until its water composition is reduced to 10% by contact with atmospheric air) could have been considered, this involves a number of environmental impacts related to nutrient pollution (Minghua et al., 2009), which it was preferable to avoid. Therefore, spent flue gas from the Rankine cycle (in combustion) and the Brayton cycle (in gasification) are used to dry the wet grape pomace. For the modeling of the drying process, it is necessary to estimate the specific heat of the grape pomace. For this purpose, the composition of grape pomace (see Table F.3 of the supplementary material) and the empirical correlation shown in the work of Sahin and Sumnu, 2006 are utilized. The concept of specific humidity and Antoine's law are added to the model to avoid gas saturation.

The combustion process, directly utilizes the dried grape pomace to produce energy by means of a furnace. To model the energy and mass balances of the combustion process, stoichiometric ratios and the empirical formula for grape pomace ($CH_{1.3626}N_{0.033}O_{0.4766}$) are used. This formula can be estimated by using the ultimate analysis of the grape pomace (Pala et al., 2014). An excess of 150% air is used to avoid too high a temperature in the furnace. By designing the furnace, it is possible to adjust the heat used to produce steam and the heat absorbed by the flue gas. This ratio is adjusted to produce enough flue gas to dry the raw material, while the remaining energy is used to produce power through the steam generated. The Rankine Cycle is modeled following the work of la Fuente and Martín, 2019.

Regarding the gasification process, the work of Sánchez et al., 2019 is followed. This process consists of grape pomace gasification, syngas upgrading and a brayton cycle. From an economic point of view, the best configuration for the gasification of lignocellulosic residues is indirect gasification (Sánchez et al., 2019) . In this type of system, the heat requirement for the gasification stage is supplied by the combustion of the char in a combustor. The heat is transferred between the combustor and the gasifier through a heat transfer medium (olivine) and the char is generated in the gasification process. Therefore, this process is autothermal. The energy and mass balances in the combustion system are performed considering the total oxidation of all compounds, except nitrogen in the air. A specific heat of combustion for char of 25000 kJ/kg is taken (Blasi, 2004). Regarding the mass and energy balances of the gasification, the composition of the outside gas is estimated using the temperature and the correlations of Phillips et al., 2007. The gasification is carried out with a pressure of 1.6 Bar and ratios of 0.4 kg of steam and 27 kg of olivine per kg of grape pomace.

The solid residues (mainly ash and olivine) are captured through a series of cyclones (99% separation efficiency) and an electrical precipitator (99.99% separation efficiency). The ZnO bed is used to separate 100% hydrogen sulfide, throught the reaction shown in Eq.(8.1).

$$ZnO + H_2S \rightarrow H_2O + ZnS \tag{8.1}$$

Subsequently, the gas is upgraded by steam reforming, removing the hydrocarbon present in the stream. Steam reforming is modeled considering that all hydrocarbons, except methane, are completely transformed into CO and H_2 (Eq. (8.2)), while the amount of CH_4 is modeled from the thermodynamic equilibrium (Roh et al., 2010) and stoichiometry ratios (Eq. 8.3 and 8.4).

$$C_nH_m + nH_2O \rightarrow nCO + (n + \frac{m}{2})H_2 \tag{8.2}$$

$$CH_4 + H_2O \longleftrightarrow 3H_2 + CO \tag{8.3}$$

$$CO + H_2O \longleftrightarrow H2 + CO_2 \tag{8.4}$$

This process is considered adiabatic. Next, the H_2/CO ratio must be adjusted to optimize the combustion process and the Brayton cycle. This process is also considered adiabatic and is modeled using thermodynamic equilibrium and Eq.(8.3) and (8.4). Finally, a PSA system is used to remove NH_3 and H_2O. Due to the selectivity of the adsorbent used in the PSA tower(zeolites), CO_2 is also adsorbed, reducing its concentration to 2%. The PSA tower is modeled using empirical performances following the literature (León & Martín, 2016). A Brayton cycle is used to produce energy because syngas is a gaseous fuel. Since the exhaust gases from the Brayton cycle are used to dry the feedstock, the use of a combined cycle is discarded. In this way, less power is produced but it is not necessary to use an external heat source to dry the grape pomace. A more detailed explanation of each process is provided in the supplementary material.

8.2.2.2 *Added-value product production*

Among the possible products that can be obtained from grape pomace, up to 3 products are considered as valued in this work. These products are biochar, fertilizer and tannins. Each product has a different production process, which are shown in Figure 8.2.

An extraction-filtration process is used to obtain tannins from grape pomace. In this case, the empirical results of the work of Ping et al., 2011 are used to estimate the mass and energy balances of this process. For the extraction process, NaOH (2.5% of the dry grape pomace), water (8:1 with respect to the solid phase) and Na_2SO_3 (2.5% of the dry grape pomace) are required. The optimum operating conditions for extraction are a temperature of 100°C and a residence time of 120 min. A filter separates the solid residue from the liquid stream, in which the dissolved tannins are found, with a ratio of 4.38 kg of liquid for each kg of solid. The liquid stream is subjected to reverse osmosis. The concentration factor of reverse osmosis for this type of product (i.e. tannins) is of the order of 7.5 (Brazinha et al., 2015). Therefore, this empirical value is used to determine

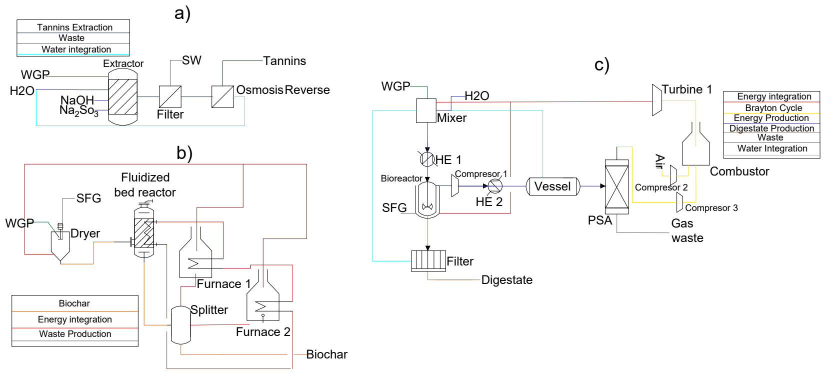


Figure 8.2: Flowcharts of processes which produce added-value products (a: Tannis, b:Biochar, and c: Fertilizer)

the maximum amount of water that can be removed from the stream, that it, and this step reduces the water content of the stream down to 13.4%. This way, much of the water used in the extraction process can be recovered. Finally the tannins are dried in contact with air to their final moisture content (9.37%) and stored. According to this work, it is possible to produce up to 0.05 grams of tannins per gram of dry grape pomace, which can be sold directly. However, a significant amount of solid residue is generated in the process (0.65 kilograms per kilogram of dried grape pomace). This residue has a composition very similar to that of grape pomace, since most of the compounds (cellulose, hemicellulose, proteins and fats) are not soluble in this solvent, and therefore, this residue can be used to produce fertilizer and biogas through an anaerobic digestion process, increasing the profitability of the process and reducing the environmental impact. The main electrical energy consumption of the process corresponds to the pumps used to reach the operating conditions of the reverse osmosis equipment, that is, 20 bar. The consumption of these pumps is estimated through an energy balance assuming an efficiency of 0.47 (Sinnot, 2005).

Fertilizer is produced by anaerobic digestion of grape pomace. The work of Taifouris and Martín, 2023 is used to model the mass and energy balances of this process. This model uses the amount of carbohydrates ($C_6H_{10}O_5$), lipids ($C_{57}H_{104}O_6$) and proteins ($CH_{2.03}O_{0.6}N_{0.3}S_{0.001}$) to estimate the composition of biogas (CH_4, CO_2, NH_3 and H_2O) using empirical biodegradability yields and stoichiometric ratios (Eq.(8.5)-(8.7)). $C_5H_7NO_2$ is the empirical formula of the cell mass.

$$\begin{aligned} &C_{57}H_{104}O_6 + 23.64H_2O + 1.4534NH_3 \rightarrow \\ &36.3665CH_4 + 13.34CO_2 + 1.45C_5H_7NO_2 \end{aligned} \tag{8.5}$$

$$\begin{aligned} &C_6H_{10}O_5 + 0.351H_2O + 0.2163NH_3 \rightarrow \\ &2.459CH_4 + 2.4592CO_2 + 0.2163C_5H_7NO_2 \end{aligned} \tag{8.6}$$

$$\begin{aligned} &CH_{2.03}O_{0.6}N_{0.3}S_{0.001} + 0.31H_2O \rightarrow 0.401CH_4 \\ &+ 0.419CO_2 + 0.036C_5H_7NO_2 + 0.001H_2S + 0.264NH_3 \end{aligned} \tag{8.7}$$

Regarding the digestate composition, it is estimated using total solids, volatile solids, total nitrogen, organic nitrogen and the potassium and phosphorus composition of the grape pomace. The process starts with a mixture of grape pomace with water up to a solids concentration of 10%. This mixture is heated to mesolphilic conditions (37ºC) and introduced into the reactor, where it remains for 21 days (Taifouris & Martín, 2018). The energy requirement of the biological reaction is often difficult to estimate from the standard enthalpy of formation of the raw materials and products. However, it can be estimated from empirical results from the work of Wu et al., 2015, and whose value is 3.4kJ/$VS_{degraded}$. The biogas is upgraded to produce biomethane using a cooling system and a PSA tower. The cooling system is modeled using Dalton's and Raoult's laws, while the PSA tower is modeled using empirical yields. The digestate is dehydrated with a centrifugal filter and stored for sale as fertilizer. The biomethane is used to produce energy through a Brayton cycle and the spent flue gas is used to supply energy to the bioreactor. Since the exhaust gases from the Brayton cycle are used to supply heat to the anaerobic digestion process, the use of a combined cycle system is discarded to avoid having to provide heat from an external source.

Biochar is produced by pyrolysis of grape pomace. First, it is necessary to dry the raw material to 10% moisture. The procedure for estimating the energy balance is the same as for the combustion and gasification processes. The pyrolysis temperature is set at 500ºC since the biochar obtained with these operating conditions presents the maximum nutrient contents (nitrogen, phosphorus and potassium) following the results of Ferjani et al., 2019. This process is modeled using the empirical yield to estimate the amount of gas (38% of the dry pomace), bio-oil (31% of the dry pomace) and biochar (30% of the dry pomace), as well as, their compositions (Ateş et al., 2019). The energy requirement is also estimated using empirical yields (Xu et al., 2009). The bio-oil and gas are used to produce energy for pyrolysis and drying of the raw material. Using the ultimate composition of the bio-oil (Ateş et al., 2019), it is possible to estimate the empirical formula, $CH_{1.33}N_{0.0316}O_{0.179}$, and model the combustion of this product. Since the gas composition is also known, modeling the combustion only requires considering the stoichiometric ratio between feedstock and products (total oxidation of all feedstock except nitrogen in the air is considered). Both flue gases are mixed to supply energy to the pyrolysis stage and to dry the feedstock. More details on each process are provided in the supplementary material.

8.2.2.3 *High-valued product production*

Through an integrated multi-product system (IMPS) it is possible to obtain polyphenols, oil and, biochar (Jin et al., 2021), following the process diagram shown in Figure 8.3. This system consists of 3 combined processes, a hexane-extraction system to produce oil, an ethanol-extraction system that uses the residues of the first one to produce polyphenols and, finally, a pyrolysis process that converts the remaining solid residues into biochar and energy. Since it is a process that integrates a large number of stages, the capital investment required is expected to be high. Therefore, grape pomace can only be used to produce oil if there is not enough capital to invest in the complete process. For this reason, the oil production process is considered as a possible independent process. Because of the wide variety of equipment used in this process together with its specific application for this type of waste, the total electricity consumption (both for the integrated system and for the oil production) is estimated from the work of Jin et al., 2021, considering a linear relationship with the grape pomace fed to the system. The electrical energy and steam required for both systems is produced through the combustion of part of the feedstock.

The seed oil is obtained by an extraction-purification process, using hexane as solvent. For this purpose, the work of Jin et al., 2021 is used as a reference. To estimate the mass and energy balances, the information on the process is used, as well as the design of the equipment shown in the supplementary material of that work. First, it is necessary to dry the raw material. Therefore, a part of the grape pomace (12.28% of the dry grape pomace) is sent to a furnace to produce flue gas, which is used to reduce the amount of water down to 7.8% moisture in the grape pomace used to produce seed oil. The seed (64%) are separated from the skins (36%) by sieving and crushing to facilitate the extraction process. The seed is fed into the extractor together with hexane (3:1 with respect to

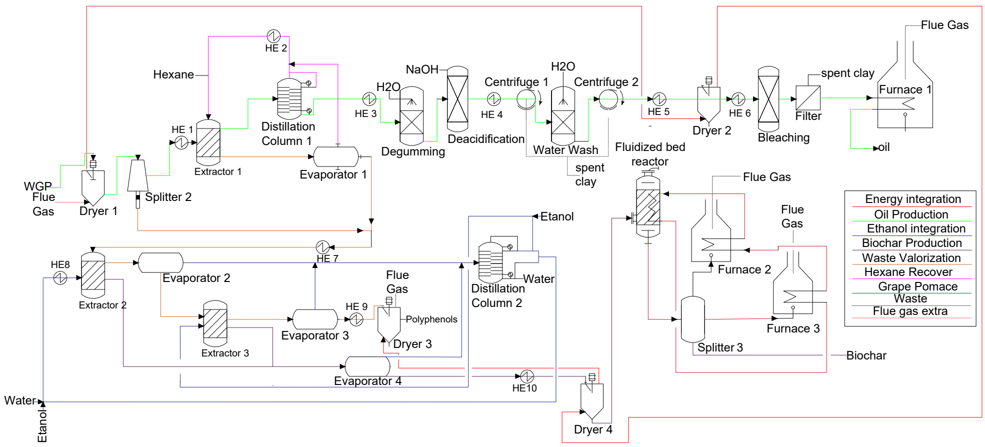


Figure 8.3: Flowchart of IMPS

the dried grape seed). This treatment recovers 98.7% of the grape seed oil. The optimun temperature of the extraction is 60ºC. After extraction, the solvent is removed in both solid (evaporation) and liquid (distillation) phases. NaOH (0.2% of the seed oil) is used for the oil deacidification phase (60ºC), while H_2O (30% of the seed oil) is added to remove the soapy fraction present in the oil. This stage is carried out at a temperature of 80ºC. The oil is dried (to 0.1% moisture) and clay (3% of the seed oil) is used to to adsorb coloring components at a temperature of 115ºC. To model the energy balance of the drying process, the specific heat of the oil is estimated following the empirical correlation of the work of Sahin and Sumnu, 2006. Finally, a furnace is used to remove odors from the oil (230ºC). However, this process presents a major drawback, since a significant amount of solid waste is generated (0.49 kg of solid waste per kilogram of dry pomace), as well as used soap and the spent clay.

The solid residues produced during seed oil production (including the skins of the grape pomace) can be sent to a new extractor that uses an ethanol solution (40% concentration) as solvent (5:1 with respect to the solids fed). This treatment recovers 82.8% of the polyphenols from the grape pomace. The optimum temperature of the extraction is 70ºC (Jin et al., 2021). A decanter centrifuge is used to separate both phases in a relation of 1.75 kg of liquid per kg of solid. The solvent is recovered by means of a two-effect evaporator. For the mass and energy balances of this stage, as well as the rest of the stages focused on ethanol recovery, the feed is considered as an ethanol-water system. Since it is possible to estimate the mass balances of this equipment from the results of the work of Jin et al., 2021 , the operating temperature of the equipment can be determined from the equilibrium data of the ethanol-water system. The temperature of this equipment is 97ºC. A decanter centrifuge and a disc centrifuge are used to separate both phases in a relation of 1.31 kg of liquid per kg of solid. All polyphenol-enriched is considered to be only recovered with the liquid phase. The polyphenol-enriched stream is subjected to a second extraction with ethanol (95% concentration) at a 2:1 ratio with respect to the feed. The solvent is recovered by evaporation (79ºC) and the stream with polyphenols is dried to 7% moisture. For modeling the evaporation and drying process, it is necessary to estimate the specific heat of the polyphenols. For this purpose, the work of Erkac and Yigitarslan, 2021 is used. As regards the solid phase, it is separated from the ethanol by evaporation and used as feedstock for a pyrolysis process, to obtain biochar and energy following the process described in section 8.2.2.2 and with the same operating conditions. The estimation of the specific heat of the solid product is necessary to model the energy balance of the evaporation process. For this purpose, the composition of the solid is considered to be similar to that of grape pomace but without the oil fraction. All streams consisting of a mixture of ethanol and water are mixed and fed to a distillation tower to obtain ethanol, with a concentration of 95 %, and water. The ethanol and water are reused in the process, reducing the economic and environmental cost of the process. More details of each process are showed in the supplementary material.

8.2.3 *Economic, environmental and social impact estimation of each process*

The economic assessment of each process is assessed using the profit, which is calculated using the income from the sale of the products and the OPEX of the processes (Eq.(8.8)).

$$Prof = \sum_{p=1}^{n} Amt_p \cdot \Pr i_p - OPEX \tag{8.8}$$

OPEX consists of a variable part (raw material cost and utilities) and a fixed part (maintenance, labor, laboratory costs, capital charges, among others). Product income and the variable part of OPEX (cost of raw material and utilities) are estimated using mass and energy balances for each process, as well as updated prices, which can be consulted in Table 8.1.

Table 8.1: Prices of the product, raw material and utilities used.

Product	**Value**	**Reference**
Power($/kwh)	0.10	(Ramos & Ferreira, 2022)
Tannins (US-$/kg)	1.50	(Sridhar et al., 2021)
Fertilizer (US-$/kg)	2.47	(Jin et al., 2021)
Biochar (US-$/kg)	2.47	
Oil (US-$/kg)	4.00	
Polyphenols (US-$/kg)	20.00	
Raw Material	**Value**	**Reference**
Grape Pomace (US-$/metric ton)	32.00	(Jin et al., 2021)
NaOH (US-$/kg)	0.41	
Etanol (US-$/kg)	0.78	
Hexane (US-$/kg)	0.9	
Water (US-$/metric ton)	0.35	
Clay (US-$/kg)	0.35	
Na_2SO_3		(ECHEMI, 2023)
Utility	**Value**	**Reference**
cooling water (US-$/metric ton)	0.05	(Jin et al., 2021)
steam (US-$/metric ton)	17.00	

The fixed part of the OPEX is estimated following the procedure shown in Sinnot, 2005. Therefore, the OPEX is calculated bt Eq.(8.9).

$$OPEX = vOPEX + Lor + \mathrm{Mn} + \mathrm{PO} + \mathrm{Lab} + \mathrm{CC} + \mathrm{Ins} \tag{8.9}$$

Where vOPEX is the variable part of the OPEX, while the rest of the costs constitute the fixed part of OPEX (fOPEX). Lor is the cost of Labor (15% of the OPEX), Mn is the maintenance (5% of the fixed capital), PO is the plant overhead (50% of the labor cost), CC is the capital charges (5% of the fixed capital), and Ins is insurances (1% of the fixed capital). Therefore, the OPEX can also be calculated as a function of the vOPEX and fixed capital, following Eq.(8.10).

$$OPEX = \frac{vOPEX + (0.11 \cdot FC)}{0.73} \tag{8.10}$$

It it necessary to calculate the CAPEX of the factory to estimate the fixed operating cost (Sinnot, 2005). CAPEX is estimated following different procedures described in the literature, depending on the process, as indicated in Table 8.2. For further details, please refer to the supplementary material.

Table 8.2: CAPEX estimation of the processes considered

Process	References
Combustion	Couper et al., 2005
Gasification	Couper et al., 2005; Almena and Martín, 2016; Sánchez et al., 2019
Anaerobic Digestion	Couper et al., 2005; Taifouris and Martín, 2023
Pyrolisis	Ramos and Ferreira, 2022
IMPS	Jin et al., 2021

Besides, the costs are updated using the CEPCI indexes (Engineering, 2022) . Once the cost of each piece of equipment has been calculated, the fixed capital cost is estimated following a factorial method described in the work of Sinnot, 2005.

In addition, the rate of return (ROR) on investment is used to analyze the profitability of each process. It is calculated following Eq.(8.11). It is assumed that the first two years there is no revenue and that taxes are of 30% (Sinnot, 2005) of the annual gross profit.

$$ROR = \frac{Comulative\ net\ cash\ flow\ at\ end\ of\ project}{Life\ of\ project\ x\ original\ investment}\ x\ 100\ per\ cent \tag{8.11}$$

The global warning potential (GWP) is used as an environmental impact index since most of the wastes generated by these processes are gaseous streams. GWP is calculated by Eq.(8.12).

$$GWP = \sum_R Amt_R \cdot Equ_R \quad \forall R \in \{CO_2, NH_3, Ethanol, SolidWaste, Steam, Soap, Water\} \tag{8.12}$$

Where Amt_R is the amount generated of each residue and Equ_R is the CO_2 equivalent. Following Eq.(8.12), the different compounds of the gaseous wastes, as well as the solid wastes generated are transformed into equivalent CO_2 using the values shown in Table 8.3.

Finally, the social impact is evaluated by analyzing job creation. Since labor cost (direct jobs) often represents between 10 and 20% of the operating cost (Sinnot, 2005) and it is estimated that 7.5 (Martín, 2016) indirect jobs are created for each direct job, the total number of jobs created by investing in grape pomace processing can be calculated using Eq.(8.13).

Table 8.3: CO_2 equivalences (Winnipeg, 2022)

Chemical (kg)	CO_2eq (kg)
CO_2	1
NH_3	2.11
Ethanol	1.24
Solid Waste	1.47E-02
Steam	0.61
Soap	1.75
Water	3.00E-05

$$Total\ J = \left(\frac{0.15 \cdot OPEX}{Sal}\right) + 7.5 \cdot \left(\frac{0.15 \cdot OPEX}{Sal}\right) \quad (8.13)$$

Where $Total_J$ is the total number of jobs created, and 'Sal' is the salary that can be estimated depending on the country where the factory is located. When direct jobs are less than 5, this equation cannot be used, since at least one person per shift is needed to maintain a continuous process. In this case, the number of direct jobs is 5 and the labor cost must be assumed to be more than 15% of the operating cost.

These indexes are normalized using the min/max method (Eq.(8.14)), to facilitate comparison between processes.

$$In_x = \frac{I - min(I_x)}{max(I_x) - min(I_x)}\ \forall x \in [Prof, GWP, TotalJ] \quad (8.14)$$

Where x consists of objective variables (profit, CO_2eq, and number of jobs), min(I_x) is the minimum value of theses variables among all of processes considered in this work, and max(I_x) is the maximum value. The impact of each index must be analyzed individually. The higher these indices are in the case of social and economic impact, the better it will be for society and for the company. However, the higher the environmental impact index, the worse it is.

8.3 RESULTS

Transportation of biomass waste is difficult due to its low density and decomposition, which increases its transportation cost and hazardousness. Therefore, the processes considered in this work are intended to be part of the winemaking process. Moreover, in this way, it is possible to better assess the amount and composition of the grape pomace, which is very important for the design and control of the waste treatment. Due to the complexity of the processes presented, especially the gasification process and IMPS, a minimum treatment capacity of grape pomace is necessary for these processes to be economically profitable. After a preliminary economic study using the models described in Section 8.2.2, it is determined that the minimum capacity is 0.1 kg/s of grape pomace for at least one of the processes to be economically profitable. For those wineries with a lower production capacity, it would be necessary to evaluate other alternatives with lower CAPEX and OPEX, such as the composting process.

Analyzing the largest wineries in California, their production ranges from 2 million cases (9-liter boxes) to 53 million cases (Downey, 2022). Therefore, these industries can generate between 18 and 477 million liters of wine per year. This is equivalent to a grape pomace production between 0.1 and 2.5 kg/s (see Section 8.2.1). The production of these wineries represents almost 40% of the total wine production in California. Therefore, if a treatment line of the grape pomace is built in all of these wineries, it is not necessary to use any type of transportation to valorize almost half of the grape pomace produced in this state of the USA. Following these production capacities, 3 sizes are considered to address the best treatment process for each type of winery, which are classified as small (0.1 kg/s of GP), medium (1 kg/s of GP) and large (10 kg/s of GP).

The optimization framework consists of eight different mathematical optimization models. Each mathematical model is optimized separately and a sensitive analysis is performed to select the best option for different capacities and investments, from economic, environmental and social points of view. An NLP is presented for each process design, which are solved on an Intel Core i7-7700 computer at 3.6 GHz (4.2GHz as turbo frequency), 65W TDP, 4 cores with 8 threads, and 32 Gb RAM (1200MHz) using GAMS.

8.3.1 *Analysis of the optimal process by type of product*

Each of the processes described in Section 8.2.2 are evaluated and optimized for the case studies described in Section 8.3 and the results are shown in Table 8.4 and Table 8.5. From the results shown in these Tables, the economic, environmental, and social impact indices are calculated for each of the processes and shown in Figure 8.4. These are used to compare each of the processes considered.

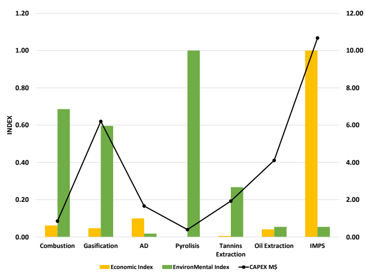
Table 8.4: Production and consumption of added-value products, raw materials, services, wastes, and energy

		Combustion	Gasification	Anaerobic Digestion	Pyrolisis	Tannins E	Oil E.	IMPS
Raw Material								
GP burnet	kg/kgGDP	0.000	0.000	0.000	0.426	0.000	0.138	0.400
Water		0.000	0.474	6.172	0.000	33.814	0.020	0.231
Na_2SO_3		0.000	0.000	0.000	0.000	0.025	0.000	0.000
Olivine		0.000	0.006	0.000	0.000	0.000	0.000	0.000
NaOH		0.000	0.000	0.000	0.000	0.025	1.01E-04	0.000
Ethanol		0.000	0.000	0.000	0.000	0.000	0.000	0.022
Hexano		0.000	0.000	0.000	0.000	0.000	0.002	0.002
Clay		0.000	0.000	0.000	0.000	0.000	0.002	0.002
Utilities								
Cooling Water	kg/kgGDP	44.513	33.116	0.852	0.000	0.113	0.169	1.144
Steam		0.000	0.000	0.000	0.000	1.217	0.029	1.834
Power	kWh/kgGDP	0.010	0.224	0.011	0.000	0.010	0.110	0.369
Waste								
Gas Waste	kg/kgGDP	18.281	10.347	3.740	12.774	3.007	2.558	6.016
Solid Waste		0.070	0.058	0.000	0.030	0.000	1.158	0.031
Products								
Power	kWh/kgGDP	0.941	3.289	0.689	0.000	0.569	0.000	0.000
Fertilizer dried	kg/kgGDP	0.0000	0.0000	0.1020	0.0000	0.0830	0.0000	0.0000
Biochar		0.0000	0.0000	0.0000	0.1370	0.0000	0.0000	0.1300
Tannins		0.0000	0.0000	0.0000	0.0000	0.0500	0.0000	0.0000
Oil		0.0000	0.0000	0.0000	0.0000	0.0000	0.0510	0.0510
Polyphenols		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0380

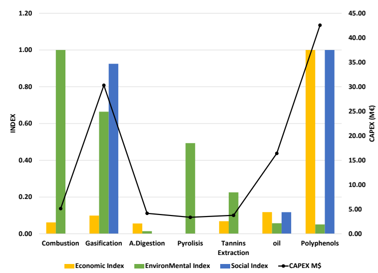
Table 8.5: Economic analysis of each process considered

		Combustion	Gasification	Anaerobic Digestion	Pyrolisis	Tannins E	Oil E.	IMPS
0.1 kg/s								
CAPEX	M€	0.849	6.200	1.661	0.395	1.926	4.288	11.077
vOPEX	M€/yr	0.007	0.187	0.005	0.000	0.126	0.010	0.164
fOPEX		0.397	0.959	0.483	0.331	0.815	0.796	1.650
Incomes		0.310	1.020	0.492	0.073	0.706	0.638	4.038
Profit		-0.094	-0.126	0.004	-0.250	-0.236	-0.168	2.224
1 kg/s								
CAPEX	M€	5.140	30.280	4.169	3.368	3.773	17.396	44.930
vOPEX	M€/yr	0.070	1.870	0.070	0.000	0.875	0.103	1.641
fOPEX		0.917	5.040	0.790	0.685	1.605	2.535	7.055
Incomes		3.101	10.200	2.764	0.727	4.907	6.383	40.380
Profit		2.114	3.291	1.904	0.126	2.425	3.746	31.684
10 kg/s								
CAPEX	M€	32.046	160.460	30.369	33.100	32.921	71.574	225.626
vOPEX	M€/yr	0.702	18.702	0.664	0.000	12.521	1.022	16.402
fOPEX		4.859	29.948	4.604	4.224	8.953	10.650	38.448
Incomes		31.012	101.996	91.325	7.273	46.914	63.828	403.810
Profit		25.452	53.337	20.161	3.882	25.440	52.156	348.960

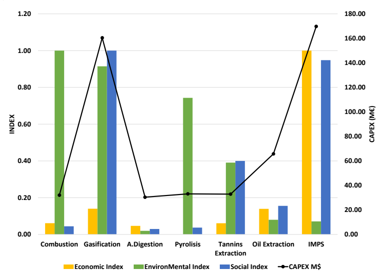
Between the energy production processes, that is, combustion and gasification, similar economic and social impacts are observed for the case of 0.1kg/s of DGP. However, the difference is larger as the capacity increases. This is due to the fact that gasification allows to produce up to 3 times more energy with the same amount of raw material and with a lower emission of greenhouse gases. This becomes even more evident in the last scenario considered (10kg/s) where economies of scale allow a much higher economic and social impact in the case of gasification. However, the process is much more complex, requiring a much higher CAPEX (5 times higher, see Figure 8.4). This also allows for a larger social impact by generating a larger number of jobs.



(a)



(b)



(c)

Figure 8.4: Economic, environmental and social impact of each process for the three capacity considered (a: 0.1 kg/s, b: 1 kg/s , c: 10 kg/s)

With respect to the added-value products, that is, the production of fertilizer, biochar and tannins, it can be observed that pyrolysis has the worst economic impact among all processes. Moreover, its environmental impact is also the highest among the processes oriented to produce chemical products. This is due to the need to dry the raw material together with the low value of the biochar. Unlike pyrolysis, anaerobic digestion does not require drying of the feedstock and allows obtaining electrical energy through biogas combustion. This has a greater economic impact than pyrolysis and tannin production for the 0.1 kg/s case. However, the economics of scale allow tannin production to have a larger economic benefit than anaerobic digestion in the 1 kg/s and 10 kg/s cases. In these cases, the best process depends on which index is given more weight, the economic or environmental impact, since tannin production has a much larger environmental impact. Although neither process requires drying of the raw material, in the case of tannin production it is necessary to burn part of the grape pomace (which produces CO_2) to generate steam to raise the temperature of the raw materials to the conditions of the extraction process (100ºC). In addition, tannin production also has a higher social impact for the 1 and 10 kg/s scenarios, given their higher CAPEX.

Finally, the oil extraction and the IMPS have the highest economic benefits among all processes (with the exception of gasification in the 10 kg/s scenario). The environmental impact is similar between both processes, being lower in the case of IMPS due to the treatment of the solid residues generated in the oil production process (see Section 8.2.2.3). In addition, the IMPS is also much better than oil extraction from the economic and social points of view. This is due to the high market value of polyphenols and the large capital investment required for their production, raising the OPEX and therefore the money available for hiring employees. Therefore, the best process to obtain high added-value products is the IMPS, analyzing any of the considered indexes. However, it should be noted that hexane extraction makes it difficult to use the oil in the food industry due to its toxicity.

8.3.2 *Analysis of the optimal process by invested capital*

The most promising process depends on three factors: the available capital for investment, processing capacity, and the weight of each index. The necessary CAPEX for each process can be consulted in Figure 8.4. Analyzing the figure, it can be observed that for all capacities, there are two processes that require much higher CAPEX than the rest, gasification and IMPS. The combustion, anaerobic digestion, pyrolysis, and tannin extraction processes have very similar CAPEX to each other and much lower than gasification and IMPS. Finally, the oil extraction process has intermediate CAPEX between the two previous groups.

If there is a large amount of available capital for investment, enough to choose between the IMPS, gasification, or oil extraction processes, then the most promising process is the IMPS, from both an economic and social point of view and for any capacity. Regarding environmental impact, only anaerobic digestion and tannin extraction (for the case of 1 kg/s) have a lower environmental impact than this process. However, the difference in economic benefit is so significant that it would be necessary to weigh the environmental impact heavily to compensate for it.

In the case that the available budget for waste treatment is insufficient to implement the IMPS or gasification process, but sufficient to select the oil extraction process, then the most promising processes are anaerobic digestion (for a capacity of 0.1 kg/s) and oil extraction (for capacities of 1 kg/s and 10 kg/s). This is mainly due to the different effects that economies of scale have on the processes. The complexity of the oil extraction process means that for small capacities, the revenues from the sale of oils do not allow for profits as high as in the case of anaerobic digestion. This allows anaerobic digestion to be the most promising process for this capacity and budget limitation. However, for larger capacities, the most promising process is oil extraction since it is better than anaerobic digestion in two indices (economic and social), better than tannin extraction in two indices (economic and environmental), and better than combustion and pyrolysis in all indices.

If the budget is even more limited, so that none of the previous three processes can be selected, the analysis becomes more complicated since the economic impacts of the remaining four processes (combustion, anaerobic digestion, pyrolysis, and tannin extraction) are very similar for capacities of 1 kg/s and 10 kg/s. For a capacity of 1 kg/s, fertilizer and tannin production are balanced, while combustion is the worst in all indices. Depending on the weight assigned to the environmental impact, one or the other is chosen as the best process due to its significant difference in this index (tannin production produces 21 times more CO2eq than anaerobic digestion). Finally, in the case of 10 kg/s, the results are similar to the previous case.

8.3.3 *Determination of optimal investment by production capacity*

A feasibility analysis is carried out to determine the best capital investment, if available, based on the profit and CAPEX of each of the grape pomace treatment processes. For this purpose, the ROR on investment of each process for each capacity is used. The results are shown in Figure 8.5.

These results show that, for the highest production case, that is, 10 kg/s, there is one process that is much more profitable than the rest, the IMPS. On the contrary, in the case of 0.1 kg/s there are several processes that are not profitable (combustion, pyrolysis, and tannin production). In this scenario, the only promising process is the IMPS. Therefore, for both capacity (0.1 kg/s and 10 kg/s), it is recommended that sufficient investment be made to implement the IMPS, provided that it is possible to do so. However, in the intermediate capacity (1 kg/s) there are several processes with very similar ROR. On the one hand, IMPS has a ROR identical to tannin extraction, but with a much higher CAPEX (5.15 times, see Figure 8.4). On the other hand, anaerobic digestion has a ROR very similar to combustion, but with

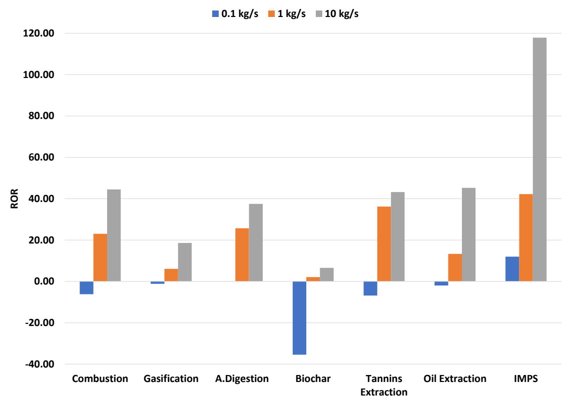


Figure 8.5: Profitability of each process for each capacity considered

a much lower environmental impact (11 times). In this case, it is better to opt for a smaller investment that involves less financial exposure.

8.4 CONCLUSIONS

This paper presents an economic, environmental and social analysis of 8 different processes for the valorization of one of the most important wastes generated during wine production, grape pomace. The processes are modeled, through mass balances, thermodynamic equilibria, empirical correlations and performances. After analyzing the economic feasibility studies, there is a strong incentive to treat these wastes to obtain added-value products, reducing the environmental impact of the wine production process and improving the social and economic impact of the entire process. The models are applied to a case study with 3 different production capacities, 0.1 kg/s, 1 kg/s and 10 kg/s.

After economic, environmental and social analysis of each of the processes, it was found that the determination of the most promising process depends on the capital invested, the production capacity of grape pomace and the weight of each of the indices that measure the economic, social and environmental impact. If sufficient capital is available, the suggested process from economic and social points of view is the integrated multi-product system, which produces polyphenols, oil and biochar, for capacities below 0.1 kg/s and above 10 kg/s. In fact, it is the only one that is really profitable for capacities below 1 kg/s. However, it is necessary to highlight that the toxicity of hexane complicates the use of the extracted oil in the food industry, opening the possibility of investigating these integrated processes for different solvents, such as supercritical CO_2 or ethanol. Only in the intermediate capacity case (1 kg/s), it may be interesting to invest in the tannin production process, if the economic and social impact are prioritized, or in anaerobic digestion, if the environmental impact is prioritized over the other two. Energy processes are discarded because they are not competitive from an economic and environmental points of view, similarly to the pyrolysis process.

It is concluded that if sufficient capital is available, the treatment of this type of waste is not only economically profitable, but also reduces the environmental impact of the wine production process, favors the circular economy of waste and has a positive social impact, generating a large number of jobs. However, for this investment to be as efficient as possible, it is necessary to select the most suitable process according to the weight of each target, the available capital and the production capacity, following the results shown in this research.

8.5 ACKNOWLEDGMENTS

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9

TOWARDS ENERGY SECURITY BY PROMOTING CIRCULAR ECONOMY: A HOLISTIC APPROACH

ABSTRACT

Dependence on fossil fuels, coupled with continuous supply disruptions by the most important natural gas suppliers, has jeopardized the energy security of most European countries. Therefore, determining the regions that can significantly increase their natural gas independence through the circular economy of their wastes is more important than ever. This work presents a multi-scale analysis to determine the possibility of implementing a circular economy toward reducing the regions dependency on fossil natural gas. A holistic approach is used to evaluate the availability of waste (manure, municipal solid waste, sludge, and lignocellulosic waste) and model the waste treatment processes (gasification and anaerobic digestion), together with a techno-economy analysis of the infrastructure required. A facility location problem optimizes the selection of the technology, the production capacity and the location of the facilities, according to the available budget. The analysis is focused on Spain, where, at the national level, an investment of 9458 M€ and an operating cost of 5000 M€ per year would allow covering 35% of the natural gas demanded. Howefver, the regional analysis shows that a total of 19 provinces can be self-sufficient with this budget. These provinces have a high biomethane production potential through lignocellulosic waste gasification and a low demand for natural gas. Since energy is a basic commodity, the ability to produce enough biomethane to cover the entire demand for natural gas gives waste valorization strategic importance at both the social and economic levels.

Keywords: Agricultural residues, Sustainable process design, Natural gas, Circular economy

RESUMEN

La dependencia de los combustibles fósiles, junto con las interrupciones continuas en el suministro por parte de los proveedores más importantes de gas natural, ha puesto en peligro la seguridad energética de la mayoría de los países europeos. Por lo tanto, determinar las regiones que pueden aumentar significativamente su independencia del gas natural a través de la economía circular de sus residuos es más importante que nunca. Este trabajo presenta un análisis a múltiples escalas para determinar la posibilidad de implementar una economía circular para reducir la dependencia de las regiones del gas natural fósil. Se utiliza un enfoque holístico para evaluar la disponibilidad de residuos (estiércol, residuos sólidos municipales, lodos y residuos lignocelulósicos) y modelar los procesos de tratamiento de residuos (gasificación y digestión anaerobia), junto con un análisis tecnológico y económico de la infraestructura requerida. Un problema de ubicación de instalaciones optimiza la selección de la tecnología, la capacidad de producción y la ubicación de las instalaciones, de acuerdo con el presupuesto disponible. El análisis se centra en España, donde, a nivel nacional, una inversión de 9458 M€ y un costo de operación de 5000 M€ por año permitirían cubrir el 35% de la demanda de gas natural. Sin embargo, el análisis regional muestra que un total de 19 provincias pueden ser autosuficientes con este presupuesto. Estas provincias tienen un alto potencial de producción de biometano a través de la gasificación de residuos lignocelulósicos y una baja demanda de gas natural. Dado que la energía es una mercancía básica, la capacidad de producir suficiente biometano para cubrir toda la demanda de gas natural otorga una importancia estratégica a la valorización de residuos a nivel social y económico.

Palabras clave: Residuos agrícolas, Diseño de procesos sostenibles, Gas natural, Economía circular.

9.1 INTRODUCTION

Notwithstanding the fact that significant efforts have been made to promote decarbonization policies among European countries (European Comision, 2018), the current dependency on fossil fuels (Martins et al., 2018), their distribution (Economides & Wood, 2009), together with potential supply disruptions of the most important suppliers of natural gas, put the energy security of most countries of the European Union at risk (Mišík, 2022). Although this risk can be reduced through a robust natural gas supply chain design (Urciuoli et al., 2014), this does not eliminate the need to import natural gas from other countries, reducing the European energy independence (Mišík, 2022).

The growing world population has led to more intensive food production systems (crops, meat, and milk, among others) (Cordeiro et al., 2022), creating areas of high organic waste production. Animal wastes, such as manure, can cause nutrient pollution, leading to the eutrophication of water bodies and soil deterioration if they are not properly treated (Menzi et al., 2009). Besides, in densely populated areas, where the production of municipal solid waste (MSW) and sludge is an issue, the treatment of this waste is quite inefficient, with 23% ending up in landfill and 26% being incinerated, losing a large part of its value (European Comision, 2021).

Both problems can be solved simultaneously by following the principles of the circular economy of the waste. Technologies such as anaerobic digestion (León & Martín, 2016) of wet waste (e.g. manure, MSW or sludge) or gasification (Sánchez et al., 2019) of dry residues (lignocellulosic waste) can provide the means to address the issue. In this context, there is a wide variety of studies focused on analyzing the biomethane production potential in different countries, such as United States (Wang et al., 2018) and Chile (Bidart et al., 2013). These studies make it possible not only to determine in which areas it is more efficient to direct waste treatment to biomethane production but also to find which of these areas can be energetically independent. This potential energy independence is an important incentive for waste treatment, due to the possibility of creating decentralized networks independent of the main pipelines (Smyth et al., 2011). This guarantees the availability of sufficient biomethane in those regions regardless of disruptions from foreign suppliers. However, most of these studies use empirical yields that directly relate biomethane production potential of a region to the number of animals, crops or people from which the residues are derived. This approach completely decouples the estimation of the amount and composition of biomethane from the transformation process and the specific composition of each waste. On the one hand, the composition of animal waste strongly depends on the feed, breed, sex, and age of the animals, which leads to large variability in the waste composition (Council, 2000). Moreover, the amount and composition of biomethane depend directly on the carbohydrate, lipid, and protein content of these wastes (Angelidaki et al., 1999). This makes it very inaccurate to estimate a biomethane production potential only considering the type of animal. On the other hand, the design of the process depends on the amount and composition of the waste, modifying the design of the equipment (size and type of equipment), as well as the production and composition of products, affecting both the economic and environmental evaluation of the process (Taifouris & Martín, 2018). Finally, the facilities must be located close to the areas where the waste is produced, due to the high economic and environmental costs associated with waste transportation (Makara & Kowalski, 2018).

A multi-scale approach allows addressing the different scales of the production system, such as physicochemical characterization of the raw material, product and process design, as well as network design and distribution, through the use of principal engineering components, such as modeling, design, synthesis, simulation, and optimization (Floudas et al., 2016). Some authors have used this approach to analyze renewable energy storage (Heras & Martín, 2021) or integrated livestock and crop management systems (Taifouris & Martín, 2022). It allows not only the adaptation of the treatment processes to the properties and amount of the waste but also the location of the facilities. This approach optimizes the treatment processes for specific cases, reducing the cost of biomethane production, as well as allowing the integration of energy between the different stages of the process. However, despite the wide variety of studies about the use of waste to produce biogas (Weiland, 2009), to the best of the authors' knowledge, there is no study that uses this holistic approach to analyze the application of the circular economy in reducing the country's dependence on fossil natural gas, as well as its operational and investment costs, the best location and size of the treatment facilities, and the optimal waste management budget.

Therefore, this work presents a study, which integrates a series of mathematical optimization models to determine, from a reduced number of parameters available in public databases, the amount of biomethane that different agricultural districts in Spain can produce from their wastes. This framework provides information on the optimal selection of treatment plants (size and type of waste treated), their location, the investment and operational costs, the production cost of the methane generated, and the percentage of consumption of CH_4 that can be covered by the biomethane produced by these factories. The main variable is the waste management budget. The rest of the document is organized as follows. Section 9.2

presents the optimization framework used to perform the proposed analysis, including a description of the problem, the procedure to estimate the amount of waste produced, the description of the processes considered to treat the waste, as well as, an explanation of the techno-economic analysis performed and the facility location problem. In Section 9.3, the model is applied to Spain, and the results are shown. Finally, in Section 9.4, the conclusions are presented.

9.2 FRAMEWORK DEVELOPMENT

To approach this study from a holistic point of view, it is necessary to consider the estimation of the amount and composition of the waste, the design of the treatment processes (both gasification and anaerobic digestion), together with the economic evaluation of its scale-up, the optimal selection of the location, and size of the facilities.

First, the framework starts by dividing the country into spatial units (provinces, counties, etc.). From the information corresponding to animal population (number of animals and their age), cultivated area, and population in each spatial unit, it is possible to estimate the amount of waste generated. Next, by modeling the gasification and anaerobic digestion processes, it is possible to establish the amount and composition of biomethane that can be produced from the composition of each of the wastes and the operating conditions of the processes. In addition, both investment and operating costs can be determined through the design of the equipment that conforms the processes. This modeling aims at determining the operating conditions to minimize the cost of biomethane production, establishing the relationship between treatment capacity, capital invested, operational costs, and biomethane produced. Since biomethane is to be injected into the country's gas installations, it is necessary that this gas complies with the technical specifications required by the country's regulations. Finally, based on the results of the previous step, a facility location problem searches for the size, type, and location of the facility that maximizes the total biomethane production for a specific budget.

9.2.1 *Estimation of the production and composition of waste*

To estimate waste production, different procedures are followed depending on the nature of the waste:

- Lignocellulosic waste: This residue is estimated from the amount and type of crops grown per year. The amount of residue grown by the type of crop can be consulted in Table 9.1. It is considered that all the waste generated is available to produce biomethane.

- Manure: The amount of manure is estimated from the number of animals and their age. 22 t/y of manure are generated by cows and calves with ages higher than 24 months, 19 t/y by calves with ages between 12 and 24 months, and 11 t/y by calves with age lower than 12 months (Merino, 2006).
- MSW and Sludge: The amount of these wastes is estimated based on the number of inhabitants of cities with a population of more than 50,000 ha. 388 kg (INE, 2019) of MSW and 105 kg (Bianchini et al., 2016) of sludge are generated per inhabitant and year in Spain.

Table 9.1: Lignocellulosic residues from crops (García-Condado et al., 2019)

Crop	Residue yield (t/ha)
Maize	8.9
Sorghum	6.4
Wheat	5.9
Rye	4.7
Oats	4.1
Barley	4.0

The most common compositions of theses residues from the literature are used, which can be consulted in Tables 9.2 and 9.3. In the case of lignocellulosic residues, an average composition has been used among the different types of residues that can be generated in crop management, since the composition varies very little from one to another. These compositions can be updated through specific studies to increase the accuracy of the estimates.

Table 9.2: Composition of the wet wastes (Alibardi & Cossu, 2015; Nielfa et al., 2015; Kafle & Chen, 2016; Park et al., 2016; Li et al., 2021; Liew et al., 2022) (RM: raw material)

Waste	**Manure**	**MSW**	**Sludge**
Unit		g/kgRM	
Lipids	0.880	1.501	0.333
Carbohydrates	17.435	38.766	2.057
Protein	3.1988	13.740	2.856
Total Solids	220	140	170
Volatile Solids	204.600	93.800	93.500
Total Nitrogen	0.229	1.159	0.144
Organic Nitrogen	0.114	0.062	0.043
Phosphorous	0.097	0.169	0.124
Potasium	0.620	0.620	0.620

Table 9.3: Ultimate analysis of the lignocellulosic waste (Wilen et al., 1996)

Component	wt% d.b.
C	47.640
H	5.835
N	0.546
S	0.106
O	41.920
Ash	3.953

9.2.2 *Process analysis and design*

In this section, the processes considered for waste treatment, the gasification of dry waste (i.e. lignocellulosic waste), and the anaerobic digestion of wet waste (i.e. manure, MSW, and sludge) are modeled. In addition, a techno-economic analysis is performed, considering 50 different waste treatment capacities for each of the wastes considered. The designs are optimized to minimize methane production costs using a non-linear program (NLP).

9.2.2.1 *Gasificacion of the biomass*

A gasification process is used for the lignocellulosic waste treatment, due to the low water content of this type of waste. The modeling of the gasification, syngas upgrading, methane production, and biomethane upgrading are based on a first principles approach, such as mass and energy balances, thermodynamic equilibrium, and empirical correlations. While a more detailed explanation of the process model is shown in the supplementary material, the most important considerations are presented below. The flowchart of the process can be seen in Figure 9.1.

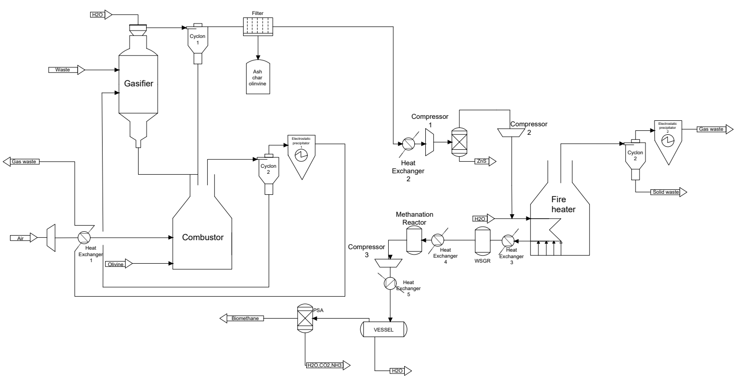


Figure 9.1: Flowchart of the biomethane production process through gasification

Following the results of Sánchez et al., 2019, the most profitable configuration is the indirect gasification system, which consists of a combination of a gasifier and a combustor (see Figure 9.1). In this type of system, the heat required for gasification is supplied by the combustion of the char formed by the gasification process (Blasi, 2004). Olivine is used as a heat transfer media (HTM) to transfer the thermal energy generated in the combustion of the char to provide the energy required for the endothermic reactions at the gasifier. In the combustor, the total combustion of all compounds is considered to perform the mass and energy balances, as well as to estimate the final temperature of this process. The composition of the syngas is estimated from the gasification temperature following the correlations of Phillips et al., 2007.

Regarding syngas upgrading, cyclones are used to separate the olivine and char. A steam reforming reactor is used to transform the hydrocarbons formed in the gasification into hydrogen. Next, a bed of ZnO is used to remove the hydrogen sulfide, with a yield of 100% (León & Martín, 2016), following the reaction presented in Eq.(9.1).

$$ZnO + H_2S \rightarrow H_2O + ZnS \tag{9.1}$$

While the cyclones and the bed of ZnO are modeled using empirical yields, the steam reforming system is modeled from the thermodynamic equilibrium conditions (Roh et al., 2010) of the two main reactions (i.e methane decomposition and the water gas shift reaction). All hydrocarbons, except for methane, are completely transformed into H_2 and CO (Aasberg-Petersen et al., 2003), following the Eq.(9.2). The amount of the rest of products and raw materials are estimated following Eqs.(9.3) and (9.4).

$$C_nH_m + nH2O \rightarrow nCO + \left(n + \frac{m}{2}\right) H_2 \tag{9.2}$$

$$3H_2 + CO \longleftrightarrow H_2O + CH_4 \tag{9.3}$$

$$CO + H_2O \longleftrightarrow H_2 + CO_2 \tag{9.4}$$

The furnace is considered as adiabatic. Subsequently, a water gas shift reactor (WGSR) is used to adjust the H_2/CO molar ratio to the optimal value for methane production in the next reactor. Equilibrium models (Roh et al., 2010) are used to relate the reaction temperature to the composition of the syngas. WGSR is also considered adiabatic. After the WGSR, an isothermal methanation (Duret et al., 2005) is used which is also modeled using mass and energy balances and thermodynamic equilibrium models (Roh et al., 2010). This reactor cannot exceed 773 K to avoid catalyst damage (Appl, 1999). Finally, a PSA system is considered to reduce the CO_2 content down to 2%, and completely remove NH_3 and water (León & Martín, 2016). This is necessary to make biomethane suitable for supply to the pipeline.

The detailed explanation of this process, together with the balances of mass, energy, and thermodynamic equilibrium, are shown in the supplementary material.

9.2.2.2 *Anaerobic digestion of the biomass*

An anaerobic digestion system is proposed to process the wastes with high water content. It is based on the work of León and Martín, 2016, and

Taifouris and Martín, 2018. Since the model of León and Martín, 2016 is not general enough to be applied to 3 different types of waste (manure, MSW, and sludge), it is necessary to develop a new model that combines both works. The flowchart of the process can be seen in Figure 9.2.

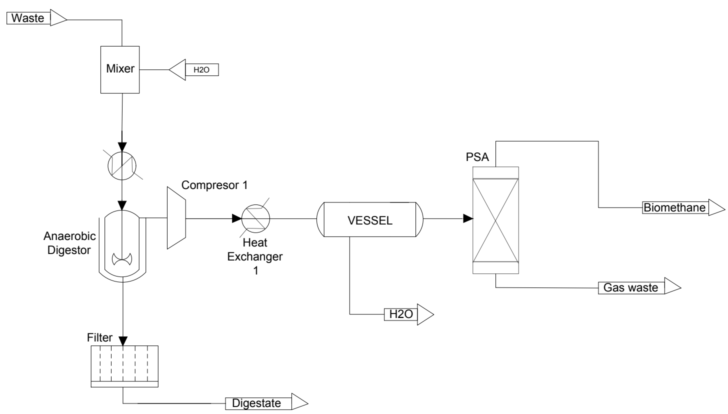


Figure 9.2: Flowchart of the biomethane production process through anaerobic digestion

León and Martín, 2016 model requires information on the amount and composition of biogas that can be obtained from a specific waste. This information is provided by the model of Taifouris and Martín, 2018 from the composition of the residues (carbohydrate, lipid, and protein fractions) using stoichiometric relationships, empirical yields, and biodegradability. The reactions of degradation of the lipids ($C_{57}H_{104}O_6$) , carbohydrates ($C_6H_{10}O_5$), and proteins ($CH_{2.03}O_{0.6}N_{0.3}S_{0.001}$) are shown by Eqs. (9.5), (9.6) and (9.7), respectively. $C_5H_7NO_2$ is the empirical formula of cell mass.

$$\begin{gathered} C_{57}H_{104}O_6 + 23.64H_2O + 1.4534NH_3 \rightarrow \\ 36.3665CH_4 + 13.34CO_2 + 1.45C_5H_7NO_2 \end{gathered} \tag{9.5}$$

$$\begin{gathered} C_6H_{10}O_5 + 0.351H_2O + 0.2163NH_3 \rightarrow \\ 2.459CH_4 + 2.4592CO_2 + 0.2163C_5H_7NO_2 \end{gathered} \tag{9.6}$$

$$\begin{aligned} CH_{2.03}O_{0.6}N_{0.3}S_{0.001} + 0.31H_2O + 0.401CH_4 + 0.419CO_2 \rightarrow \\ +0.036C_5H_7NO_2 + 0.001H_2S + 0.264NH_3 \end{aligned} \tag{9.7}$$

Using the information from the model of Taifouris and Martín, 2018, together with a series of physical-chemical parameters of the residues (total solids, volatile solids, carbon content, etc.), the model of León and Martín, 2016 can adjust the distribution of the different gases (mainly H_2O, NH_3, and CO_2) between the gaseous (biogas) and the liquid phases (digestate). In addition, this new model allows estimating the amount of nutrients (nitrogen, potassium, and phosphorus) that the liquid/solid effluent of the bioreactor has, crucial information to evaluate the usefulness of the digestate produced.

The biogas is purified by using a bed of iron, to remove the H_2S, and a PSA system to reduce their CO_2, NH_3, and H_2O content to achieve an acceptable biomethane composition. The detailed explanation of this process, together with the balances of mass and energy, the thermodynamic models, and empirical yields, is shown in the supplementary material.

9.2.2.3 *Techno-economic analysis and process scale-up*

A process is designed for each type of waste, as described in Sections 9.2.2.1 and 9.2.2.2, together with the corresponding operational expenditure (OPEX) and capital expenditure (CAPEX), modeling up to 50 designs with different waste treatment capacity. The sizes range from a minimum size, which depends on the minimum amount of waste available considering all the space units of a country; and a maximum size that is fixed by references (Rico, 2020) (for wet residues) or the maximum waste available considering all spacial units (for lignocellulosic waste). Each of these designs is optimized through an optimization model whose objective function is to reduce biomethane production costs.

For the OPEX, both fixed and variable costs are estimated, following the procedure described in Sinnott, 2005. The cost of waste is not considered because it is produced at the same place where it is treated and has no market value so far. However, the auxiliary costs (steam, water, and energy) are considered and determined from the mass and energy balances carried out for each of the processes. In addition to these costs, labor, maintenance, laboratories, depreciation, and insurance (all fixed costs) are estimated following the procedure of Sinnott, 2005.

Regarding CAPEX, the first step is to estimate the cost of the equipment. Each piece of equipment that constitutes the processes of anaerobic digestion and gasification is analyzed, as well as its size and its cost estimation. For the economic estimation of the reactors, the bed of ZnO, as well as the indirect gasifier, the procedure described in the work of Sánchez et al., 2019 is used. The compressors, heat exchangers, and the fire heater are designed following the correlations shown in the work of Couper et al., 2005, while the electrostatic precipitator, filters, and cyclones are designed based on the studies of Almena and Martín, 2016. The digester is designed following the work of Taifouris and Martín, 2018. Once the cost of equipment is estimated, the rest of the capital costs (equipment erection, instruments, process buildings, and structures, among others), necessary for the construction and start-up of the factories, can be calculated following a factorial method, which is shown in Sinnott, 2005. For more information on economic estimation, please consult the supplementary material.

9.2.3 *Facility location problem*

Following the results from the previous stages, an extended location problem is formulated to select the number, size, type, and location of facilities, between the 50 possible designs. It is a mixed-integer linear programming (MILP) that aims at maximizing the total biomethane production for a specific budget. Binary variables are used for plant selection. First, it is necessary to determine the amount of biomethane (Biomet$_p$) that can be produced in each spatial unit 'p'. This depends on the number of each type of factory (each design 'q' of each kind of waste 'w') installed in each spacial unit 'p' (Nfact$_{w,q,p}$) and its biomethane production (CH4fact$_{q,w}$), by using Eq.(9.8).

$$Biomet_p = \sum_w \sum_q Nfact_{w,q,p} \cdot CH4fact_{q,w} \quad \forall p \tag{9.8}$$

CH4fact$_{q,w}$ is obtained as a result of the previous stages.

Since the plants installed in a spatial unit 'p' cannot consume more waste than is available at that location, it is necessary to estimate the total waste treated by all of the installed plants in a spatial unit 'p' (Wst$_{w,p}$) through Eq.(9.9).

$$Wst_{w,p} = \sum_q Nfact_{w,q,p} \cdot Wastefact_{q,w} \quad \forall w \tag{9.9}$$

Where Wastefact$_{q,w}$ is the treatment capacity of a plant with the design 'q' treating the waste 'w'.

Regarding OPEX and CAPEX of all waste treatment plants installed in a spacial unit 'p' (CstO$_p$ and CstF$_p$, respectively), they are estimated by Eqs.(9.10)-(9.11), respectively.

$$CstO_p = \sum_w \sum_q Nfact_{w,q,p} \cdot COfact_{q,w} \;\; \forall p \tag{9.10}$$

$$CstF_p = \sum_w \sum_q Nfact_{w,q,p} \cdot CFfact_{q,w} \ \ \forall p \tag{9.11}$$

Where OPEX and CAPEX of each of the different designs 'q' for each of the different wastes 'w' (COfact$_{q,w}$ and CFfact$_{q,w}$) are obtained by following the procedure described in Section 9.2.2.3. Thus, the total OPEX (Topex) and the total CAPEX (Tcapex) are calculated by Eqs.(9.12)-(9.13). Transportation costs are not considered since it is expected that the facilities are located near the areas with a high waste production, due to the high economic and environmental costs associated with waste transportation (Makara & Kowalski, 2018). Therefore, this cost will be negligible compared to the COPEX and OPEX of the factories.

$$Topex = \sum_p \operatorname{Cos} tO_p \tag{9.12}$$

$$Tcapex = \sum_p \operatorname{Cos} tF_p \tag{9.13}$$

Topex must be less than the selected annual budget (Eq.(9.14)).

$$Topex \leq Annual \ \ Budget \tag{9.14}$$

With the selected budget, the fraction of natural gas demanded that can be covered by biomethane (fcov$_p$), in each spacial unit 'p', is given by Eq.(9.15), while the total fraction covered (Tfra) is estimated by Eq.(9.16).

$$f_{\mathrm{cov}_p} = \frac{Biomet_p}{Ngas_p} \quad \forall p \tag{9.15}$$

$$Tfra = \frac{\sum_p Biomet_p}{\sum_p Ngas_p} \tag{9.16}$$

9.3 RESULTS

9.3.1 *Case of study*

The optimization framework presented in previous sections is applied to analyze the reduction of fossil natural gas dependence in Spain toward the circular economy of its waste. The country is divided into agricultural districts, that is, 345 possible locations. Among the different countries of the European Union, Spain has been selected for three reasons. It has a large agro-industrial production (Gobierno de España, 2022), and therefore, a large production of waste. In addition, Spain is highly dependent on foreign natural gas suppliers (Enagas, 2022). Finally, the current production of biomethane is quite limited compared to other countries (European Biogas Association, 2021).

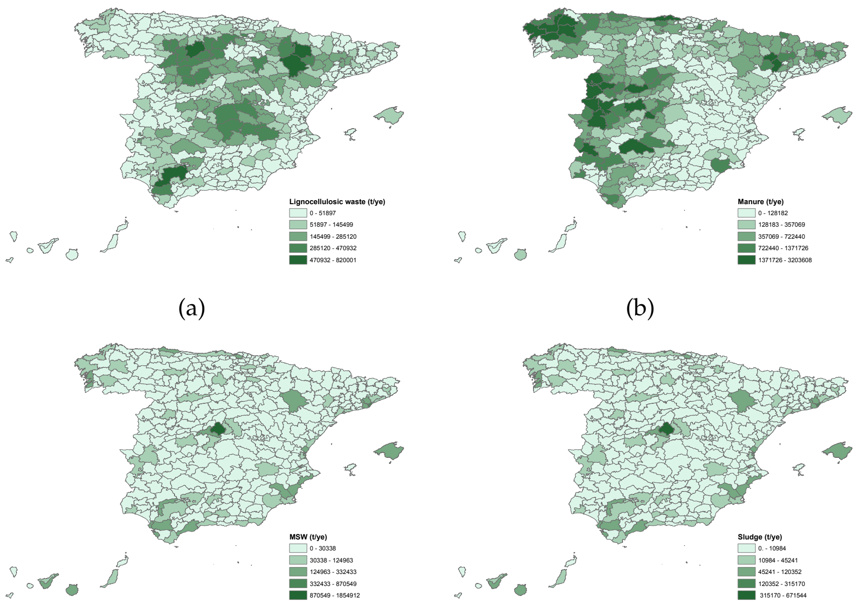
Regarding waste production, Figure 9.3 shows the spatial distribution of lignocellulosic waste (a), manure (b), MSW (c), and sludge (d), in Spain. Lignocellulosic residues are estimated from annual crop data (Escudero et al., 2021). Manure is estimated from animal census and age distribution (Instituto nacional de estadistica, 2021), while that MSW is calculated from the population of all cities with more than 50,000 inhabitants. In those agricultural districts that have more than one city with these characteristics, their MSW production is added, while in those that only have cities with less than 50,000 inhabitants, their MSW production is assumed to be 0.

The consumption of natural gas can be seen in Figure 9.4. This consumption can be estimated from reports (Comisión Nacional de los Mercados y la Competenicia, 2021). The technical specifications of the biomethane obtained must comply with the specifications indicated in the reference (Ministerio para la Transción Ecológica, 2018).

Finally, the optimization framework used for this study consists of two different type of mathematical optimization model. A NLP for each process design, and a MILP for facility location problem, which are solved in an Intel Core i7-7700 computer at 3.6 GHz (4.2GHz as turbo frequency), 65W of TDP, 4 core with 8 threads, and 32 Gb of RAM (1200MHz) by using GAMS.

9.3.2 *Properties of the different types of factories*

As explained in Section 9.2.2.3, 50 different factories, with different production capacities, are designed and optimized for the treatment of the wastes considered, based on the characteristics of the regions considered in this case of study. These spatial units determine the maximum and minimum size of these factories. Once designed, following the procedure described in Section 9.2, the waste processing capacity, methane production, as well as OPEX, and CAPEX to build them can be determined. The most relevant data are shown in Table 9.4. Although the relationship between biomethane production and treatment capacity of the plant is linear with the treatment capacity, the production cost of biomethane



(a) (b)

(c) (d)

Figure 9.3: Amount of (a) lignocelulosic wastes, (b) manure, (c) MSW and (d) sludge

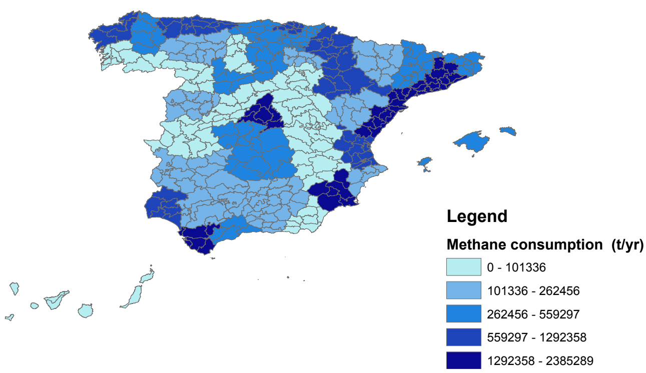


Figure 9.4: Consumption of natural gas in each agricultural district

follows a power law. This is due to the strong economy of scale since a large part corresponds to fixed costs, above 90%.

Table 9.4: Main results of the techno-economic analysis of the residues (q: capacity of factory(t/y), WW: wet waste).

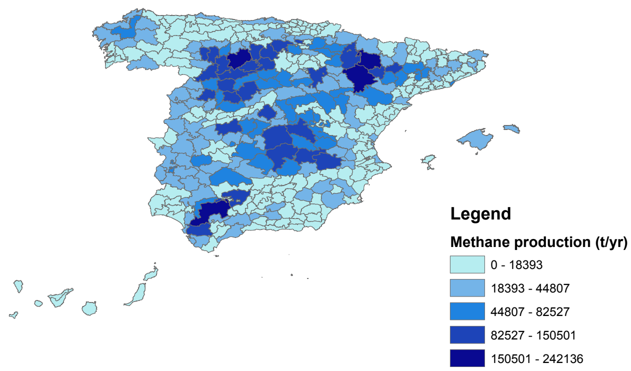
Residue	Yield ($kg_{biomethane}/kg_{WW}$)	Production Cost (€/kg_{WW})	Minimum Capacity(t/y)	Maximun Capacity(t/y)
SLUDGE	0.003	Pcost= $1814278231 \cdot q^{-0.97}$	700624	49754
MANURE	0.012	Pcost = $160365047 \cdot q^{-0.885}$	63072	367920
MSW	0.070	Pcost = $72035915 \cdot q^{-0.97}$	19657	52560
LIGNO	0.285	Pcost = $606041 \cdot q^{-0.626}$	10000	820000

9.3.3 *Total potential of biomethane production in Spain*

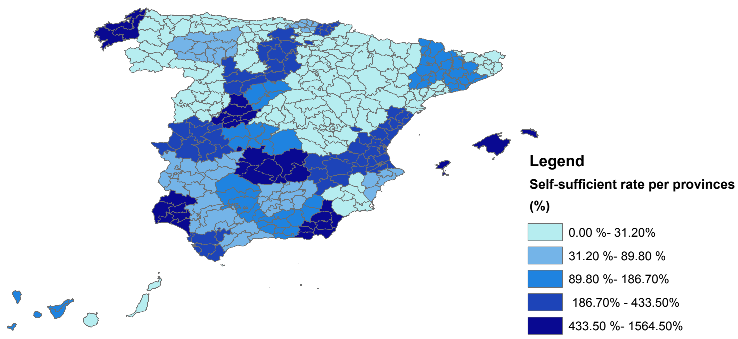
The results show that 43% of natural gas consumed could be supplied through the treatment of the available wastes. However, this requires a total CAPEX of 21391M€, as well as an OPEX of 25852M€ per year. In order to obtain these results, the process design is optimized to maximize biomethane production at each spot, but the localization of the plant is not optimized, as it aims at treating all available waste.

The maximum amount of biomethane that can be produced in each agricultural district is shown in Figure 9.5a. If this distribution is compared with the amount of residues (Figure 9.3), it can be observed that the production of biomethane is consistent with the distribution of lignocellulosic waste. This is because most of the biomethane is produced from lignocellulosic waste by using gasification. This technology has a yield of 28.5% (28.5 kilograms of biomethane are generated per 100 kilograms of biomass) while manure, MSW, and sludge have yields of 1%, 7%, and 0.3%, respectively (see Table 9.4). The large difference between these yields is due to the composition of the waste and the technology used to produce biomethane. Manure, MSW, and sludge use anaerobic digestion, while lignocellulosic waste uses gasification. For this reason, although the amount of residues is larger in the cases of wet waste, the amount of biomethane generated from lignocellulosic wastes is larger (8250 kt/y vs 2103 kt/y).

By analyzing the fraction of natural gas demand satisfied by using biomethane (see Figure 9.5b), there is a total of 21 provinces that would be totally independent of natural gas with this capital investment. Some of those that have a higher level of independence include 'La Coruña', 'Ávila', 'Ciudad Real', 'Almería' , 'Huelva', and 'Baleares'. In addition, there is an important mismatch between large industrial zones, urban areas, and the main cultivation regions. It is responsible for that difference between production and demand (see Figure 9.3 and 9.4). The demand is highly centralized in provinces such as 'Madrid', 'Barcelona', 'Asturias', 'Murcia', and 'Cadiz'.



(a)



(b)

Figure 9.5: Potential biomethane production (a) per agricultural district and demand for natural gas that it could satisfy per province (b)

9.3.4 *Determination of the optimal budget for the reduction of Spain's dependence on fossil natural gas*

The facility location problem is used to optimize the selection of the size, type, and location of the facilities for different available budgets. This allows drawing the Pareto curve (Figure 9.6) between the self-sufficiency ratio and the selected waste treatment budget. The self-sufficiency ratio is defined as the ratio of biomethane produced to methane consumed and is not linear. As can be seen in Figure 9.6, there are two sections, divided by the point of 5000 M€ per year. In the first section, there is an increase of 2% in the self-sufficiency rate per 100M€ spent, while in the second section, the self-sufficiency remains almost constant (0.02% per 100M€ used). Therefore, the point of 5000 M€/year is selected as the best budget to spend on the construction of waste treatment plants in Spain. This OPEX corresponds to a CAPEX of 9505M€.

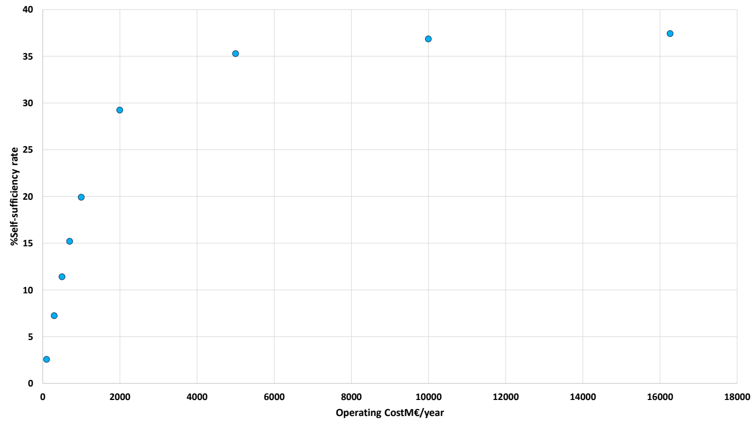
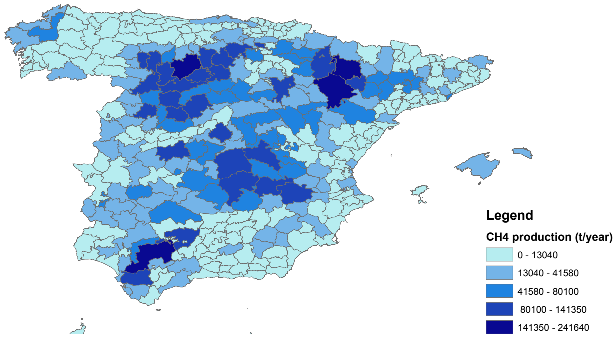


Figure 9.6: Relation between the budget for operating cost and the self-sufficiency rate

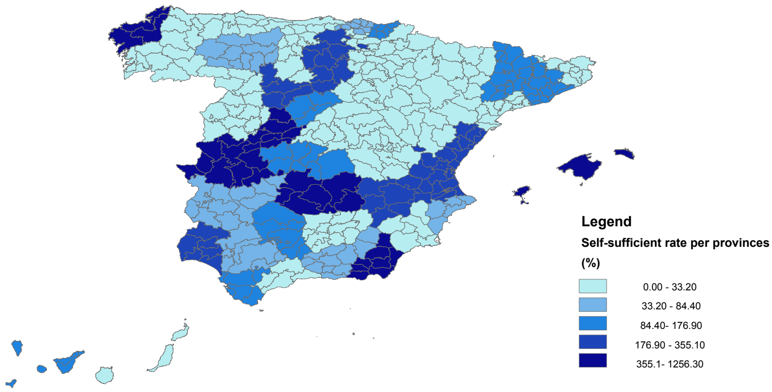
For this budget, the amount of biomethane generated by the agricultural district can be seen in Figure 9.7a. This corresponds to 206 lignocellulosic waste , 141 manure, 148 MSW, and 0 sludge treatment plants , which can be seen in Figures 9.8 and 9.9 . With this distribution of treatment plants, it is possible to cover 35% of the country's total natural gas demand, and 19 provinces are totally independent of natural gas from foreign suppliers. These provinces correspond mostly to rural areas, which have a higher concentration of lignocellulosic residues or manure, that is, greater potential for natural gas production and less access to the main gas pipelines.

From techno-economy analysis of the plants, it is observed that 90 % of the operating costs corresponds to fixed costs (labor, maintenance, capital charges, and insurance) while the remaining percentage corresponds to variable costs (raw material, auxiliary services, and energy) in the case of gasification factories.

In anaerobic digestion processes, this distribution is even more uneven, with 99% versus 1%. Since plant size does not have a high effect on operational costs, the economy of scale is even more favored, pushing the selection of plant size to the maximum allowed in each of the selected agricultural districts. In the case of wet waste treatment (MSW and manure), larger designs are selected (above 35,000 tons per year for manure and 50,000 tons per year for MSW), representing 97% of the designed plants. In the case of dry waste, the plants are much larger and in most of the selected agricultural districts, there is not so much waste available for factories of those sizes. Therefore, the most selected plants are small



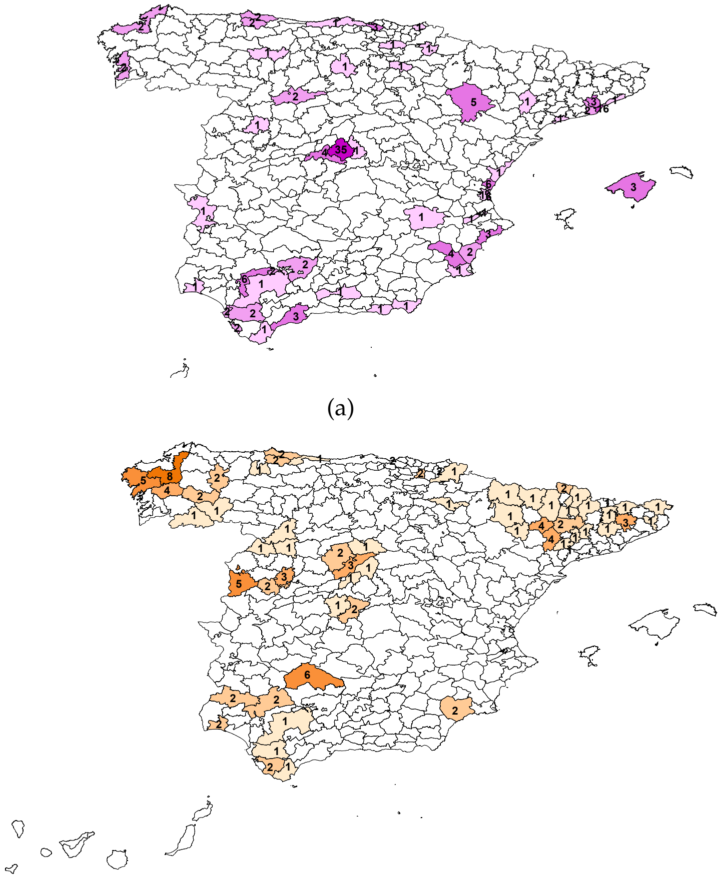
(a)



(b)

Figure 9.7: Production of Biomethane (ton/year) with a budget of 5000 MM€/year (a) and self-sufficient rate of each provinces (b)

(below 50,000 tons/year), representing 50% of the selected plants. 5000 M€ represents 40.6% of the budget of the Ministry for Ecological Transition and the Demographic Challenge (MITECO) in 2021 (Ministerio para la transición ecológica y el reto demográfico, 2020). Considering the OPEX and the total amount of biomethane produced, the unit cost of biomethane is 34.8 €/MWh or 10.19 USD/MMBTU. Since this study is addressing a feasibility analysis, the margin of error of the biomethane cost estimate is 30% (Sinnott, 2005). Therefore, this cost is between 7.13 and 13.25 USD/MMBTU and is below the current price of natural gas in Europe (39.02 USD/MMBTU) (World Bank, 2022)



(a)

(b)

Figure 9.8: Factories for the treatment of manure(c) and msw(d)

Finally, it is important to highlight that, as in the results shown in Section 9.3.3, there is a significant mismatch between the regions that demand natural gas and the districts that generate biomethane (see Figure 9.7b).

9.4 CONCLUSIONS

Due to the energy dependence of European countries on foreign natural gas suppliers, any disruption in delivery could affect the energy security of a large number of countries. Because of this, together with the environmental problems associated with the generation of waste, it is essential to make the best use of the waste generated by both industry and the population. This work presents a multiscale and holistic analysis to assist in the

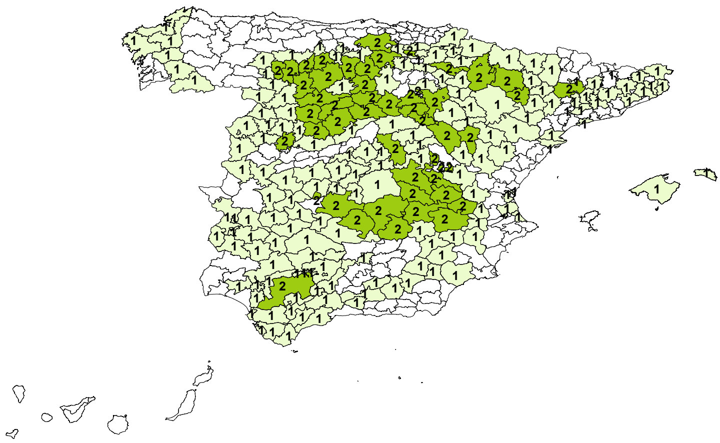


Figure 9.9: Factories for the treatment of lignocelulosic wastes

decison-making process regarding waste treatment. It integrates a series of mathematical models that allow estimating the amount of biomethane that a country can produce, what is the best process and waste for it, the cost and location of the plants, taking into account the number of animals, the annual crop production, and the population of large cities, as well as the available budget.

As regards its application to the specific case of Spain, it was determined that almost half of the natural gas consumed could be produced by treating the total waste available. By comparing the maximum biogas production potential with the optimal valorization of the available wastes, the results show that it is possible to reduce the total CAPEX and OPEX of the waste treatment plants down by 57.92% and 80.65% respectively, while the percentage of natural gas covered by biomethane was reduced by only 19% percent. Therefore, it is concluded that the point of greatest profitability is reached at 5000 M€ per year of operational costs.

This OPEX is of the order of the budget that is being allocated annually for MITECO. The government invests this budget in the elaboration of various plans for the improvement of water quality, waste treatment and sustainable energy production (Ministerio para la transición ecológica y reto demográfico, 2022b). Among these plans, it has recently developed a specific plan to increase the country's energy security, for which this type of analysis is paramount (Ministerio para la transición ecológica y reto demográfico, 2022a). With this OPEX, 19 provinces can be independent of natural gas from foreign suppliers. Since the gas supply is assured between these provinces, the development of decentralized structures can be taken into account, reducing the stress on the central pipelines. Moreover, by producing the natural gas at the site of consumption, the environmental and economic impacts are reduced by avoiding the necessary transportation between the points of consumption and the nearest pipeline. Therefore, this can be a strong incentive to create energy policies focused on prioritizing the construction of waste treatment plants oriented to biomethane production in these specific areas. From the results of the analysis, it is also concluded that the most cost-effective process is gasification, so the treatment of lignocellulosic waste is prioritized over other wet wastes. This means that most of the plants are located close to the large cultivation areas, that is, around the center of the country.

This analysis is easily applicable to other countries, simply by changing the databases. In addition, certain physicochemical parameters, such as waste composition, can be adjusted for particular cases, in order to improve the estimates, without affecting the procedure described in this work.

Finally, as society moves towards a zero-carbon energy production system, these plants can be easily adapted to produce green hydrogen (Antonini et al., 2020), which can be use either as a fuel or raw material to produces other chemical products.

9.5 ACKNOWLEDGMENTS

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10

CONCLUSIONS

Integrated process and product design and the addition or extension to include the supply chain present a number of challenges. They must be approached from a multiscale approach, the core of which presents significant mathematical issues, such as nonlinear terms and large sizes.

This thesis has identified them and several strategies are proposed to address these problems. Extended pooling and food formulation problems result in large MINLP ones. To address such complex models, a number of techniques have been developed including the substitution of binary variables by continuous variables for the decision-making processes, multistage optimization, sensitivity studies to establish limits on the variables, and some linearization-decomposition of the problem. In addition, multi-objective and multi-period optimization models have been used to analyze the selection of products, processes, and supply chains from different points of view (economic, environmental, and social). In addition, the production of added-value products from waste valorization was also analyzed. The large portfolio of alternative products and technologies claims a systematic approach that conbines heuristics for preselection and mathematical optimization for the design of the process and the selection of the products. The exploitation of residues across a large region represents a multiscale problem. The selection of the technologies and their size required the analysis of the processes and the formulation of a facility location problem that can capture the effect of the distributed availability of residues.

From the application of these techniques to different case studies, the following conclusions have been obtained, which respond to the objectives set out at the beginning of this thesis:

- The result of applying a decomposition/linearization algorithm to the integrated product, process, and supply chain design for detergent powder production shows that specialization by product type is the best strategy, as it takes advantage of economies of scale and reduces transportation costs.

- By analyzing the integration of product design, process, and supplier selection from an economic and environmental point of view it is possible to find a formulation for a detergent powder that reduces the environmental impact of its production and distribution by 40%, compared to its design based on purely economic objectives, without significantly affecting the profitability of the operation.

- The integration of the meat and crop production process through the optimal formulation of animal feed allows for the reduction of the environmental impact by up to 62% of the environmental impact produced, compared to the decoupled meat and feed production system. This reduction is mainly due to the selection of crops with lower fertilizer consumption. However, a lower economic benefit can be obtained from the sale of these crops, which represents a loss of profit of 14% compared to the decoupled systems. A program of subsidies aimed at increasing the sustainability of food production processes could be proposed to compensate for these losses in benefits.

- Adding sizing and location to the design of integrated meat production and crop management systems allows for a holistic approach to the design of these types of food production systems as they jointly affect the environmental impact and economic performance of the farm. The difference in crop growth performance depending on location can reduce the economic benefit down to 3 times. In addition, there are a number of locations that are particularly sensitive to nitrate release or are protected as nature reserves, which reduces the number of possible locations by 42%. Since the multi-objective (economic and environmental) optimization model has a large number of decision variables (feed design, crop selection, nutrient recovery, fertilizer formulation, location, and size), the environmental impact can be reduced by 35%, with respect to the purely economic optimization scenario, without greatly affecting the economic benefit. Although the largest cost item is associated with crop production (34.10%), the main business activity of the integrated system is crop production. Finally, the production cost of meat from this type of integrated systems is 8.87 €/kg, of which 1.61 €/CB corresponds to the cost of waste treatment. However, the cost of meat from this work can be reduced, if the income from the harvests sold is taken into account, to 1.51 €/CB.

- Analyzing together the composition of the spent coffee grounds (SCG) and the possible valorization processes for this type of waste, it was concluded that the most profitable process from an economic point of view was the production of natural pigments. In spite of the fact that the most valuable product that can be obtained from this residue is the natural caffeine extract, its concentration in this residue is much lower than the amount of natural pigments that can be obtained, which allows the income from the sale of natural pigments to be almost 4 times greater than the income from the sale of the natural extract. Energy production by SCG combustion is much less profitable and aerobic digestion is not profitable due to the high cost of digesters.

- By jointly analyzing the composition of grape pomace together with its possible treatment processes, it was concluded that the valorization of this waste is not only economically profitable but also reduces the environmental impact of wine production by favoring the circular economy of its residues and has a positive social impact by allowing the generation of jobs. The optimal selection of the process, in addition to the composition of the waste, depends on the processing capacity of the facility and the weight given to each objective (economic, social, and environmental). If the capacity is less than 0.1 kg/s or more than 10 kg/s, the best process from an economic and social point of view is one that simultaneously produces essential oils, polyphenols, and biochar. However, for intermediate capacities, tannin, and digestate production may be selected as the optimal processes depending on the weight assigned to each objective. Energy recovery processes are discarded as they are not competitive from an economic or environmental point of view.

- By treating all the agricultural and human waste generated in a year in Spain, it is possible to produce biomethane to compensate for up to almost half of the natural gas consumed. By analyzing the composition of the waste, its biodegradability, and its conversion into biomethane, it is concluded that the best process to produce biomethane is the gasification of lignocellulosic waste. Therefore, if the budget is limited, the construction of lignocellulosic waste gasification plants will be prioritized over the anaerobic digestion of manure, municipal solid waste, or sewage sludge. Due to the large difference in performance between gasification and anaerobic digestion, there is an optimal annual budget for waste treatment, which in the Spanish case is 5,000M€. With this budget, up to 19 provinces can be economically independent, which is a strong incentive due to the social and economic importance of energy security in rural areas. If a higher budget is established, it is invested in the operation of anaerobic digestion plants that do not significantly increase the country's self-sufficiency coefficient (0.02% for every 100 million euro increase in the budget) and therefore is no longer economically profitable.

Part III

APPENDIX

A

APPENDIX A: SUPPLEMENTARY INFORMATION OF CHAPTER 3

The tables, which are used in the case of study and they were not included in the manuscript, are attached below:

Table A.1: Maximum available amount of the raw material (Martín & Martínez, 2018)

Supplier/Ingredient(t)	1	2	3	4	5	6	7	8	9	10	11	12	13
LAS	0	0	0	400	400	400	0	0	0	0	0	0	0
AE	0	0	0	400	400	400	0	0	0	0	0	0	0
MTEA	0	0	0	400	400	400	0	0	0	0	0	0	0
STPP	500	500	500	0	0	0	0	0	0	0	0	0	0
Zeolite	500	500	500	0	0	0	0	0	0	0	0	0	0
Sodium perborate	250	250	250	0	0	0	0	0	0	0	0	0	0
Sodium percarbonate	250	250	250	0	0	0	0	0	0	0	0	0	0
Sodium sulfate	200	200	200	0	0	0	0	0	0	0	0	0	0
Xylene sulphonate	200	200	200	0	0	0	0	0	0	0	0	0	0
Antifoan	0	0	0	50	50	50	0	0	0	0	0	0	0
Protease	0	0	0	0	0	0	30	30	30	30	30	30	0
Lipase	0	0	0	0	0	0	30	30	30	30	30	30	0
Cellulose	0	0	0	0	0	0	30	30	30	30	30	30	0
Carboxymethyl cellulose	0	0	0	20	20	20	0	0	0	0	0	0	0
Sodium polyacrylate	0	0	0	20	20	20	0	0	0	0	0	0	0
Polietilen glicol	0	0	0	20	20	20	0	0	0	0	0	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	500

Table A.2: Minimum available amount of the raw material (Martín & Martínez, 2018)

Supplier/Ingredient (t)	1	2	3	4	5	6	7	8	9	10	11	12	13
LAS	0	0	0	0	0	0	0	0	0	0	0	0	0
AE	0	0	0	0	0	0	0	0	0	0	0	0	0
MTEA	0	0	0	0	0	0	0	0	0	0	0	0	0
STPP M1	0	0	0	0	0	0	0	0	0	0	0	0	0
Zeolite	0	0	0	0	0	0	0	0	0	0	0	0	0
Sodium perborate	0	0	0	0	0	0	0	0	0	0	0	0	0
Sodium percarbonate	0	0	0	0	0	0	0	0	0	0	0	0	0
Sodium sulfate	0	0	0	0	0	0	0	0	0	0	0	0	0
Xylene sulphonate	0	0	0	0	0	0	0	0	0	0	0	0	0
Antifoan	0	0	0	0	0	0	0	0	0	0	0	0	0
Protease	0	0	0	0	0	0	0	0	0	0	0	0	0
Lipase	0	0	0	0	0	0	0	0	0	0	0	0	0
Cellulose	0	0	0	0	0	0	0	0	0	0	0	0	0
Carboxymethyl cellulose	0	0	0	0	0	0	0	0	0	0	0	0	0
Sodium polyacrylate	0	0	0	0	0	0	0	0	0	0	0	0	0
Polietilen glicol	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0

Table A.3: Size of the intermediate tanks (Martín & Martínez, 2018)

Tank	Size (m^3)
1	300.5
2	300.5
3	300.5
4	300.5
5	300.5

Table A.4: Maximum demand per year (Martín & Martínez, 2018)

Year/product (t/yr)	1	2	3
1	300	400	100
2	300	400	100
3	300	400	100

Table A.5: Minimum demand per year (Martín & Martínez, 2018)

Year/product(t/yr)	1	2	3
1	200	100	50
2	200	100	50
3	200	100	50

Table A.6: Composition of ingredient k in the flow (Martín & Martínez, 2018)

t_i/t_k	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
LAS	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AE	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MTEA	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
STPP M1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Zeolite	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Sodium perborate	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
Sodium percarbonate	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
Sodium sulfate	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
Xylene sulphonate	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
Antifoan	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
Protease	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
Lipase	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
Cellulose	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
Carboxymethyl cellulose	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
Sodium polyacrylate	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
Polietilen glicol	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Table A.7: Maximum concentration of the group of ingredients g in the product j (Martín & Martínez, 2018)

t_i/t_j	1	2	3	4	5	6	7	8
1	0.250	0.600	0.250	0.500	0.050	0.050	0.050	0.500
2	0.250	0.600	0.250	0.500	0.050	0.010	0.050	0.500
3	0.250	0.600	0.250	0.600	0.050	0.010	0.050	0.500

Table A.8: Maximum concentration of the group of ingredients g in the product j (Martín & Martínez, 2018)

t_i/t_j	1	2	3	4	5	6	7	8
1	0.150	0.100	0.050	0.100	0.001	0.001	0.001	0.005
2	0.150	0.100	0.050	0.100	0.001	0.001	0.001	0.005
3	0.150	0.100	0.050	0.100	0.001	0.001	0.001	0.005

Table A.9: Equivalent CO2 emission (Fawer et al., 1998; Patel et al., 1999; Kowalski et al., 2010; Althaus et al., 2017; Ecoinvent, 2019)

Ingredient	kg_{CO2}/kg_{ingr}
LAS	4.20
AE	3.70
MTEA	4.0
STPP	1.02
Zeolita	1.76
Sodium perborate	0.40
Sodium percarbonate	0.40
Sodium sulfate	0.30
Xylene sulphonate	0.03
Antifoan compound	1.76
Protease	3.69
Lipase	3.69
Cellulose	3.69
Carboxymethyl cellulose	2.22
Sodium polyacrylate	0.02
Polietilen glicol	0.17
Water	0.00

Table A.10: Prices without discounts

Ingredient (€/kg)	1	2	3	4	5	6	7	8	9	10	11	12	13
STPP	0.039	0.048	0.054	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ZE	0.021	0.030	0.036	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
S. PERBO	0.210	0.300	0.360	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
S. PERCA	0.210	0.300	0.360	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
S.SU	0.021	0.030	0.021	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
X.SU	0.042	0.060	0.042	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PRO	0.000	0.000	0.000	0.000	0.000	0.000	3.900	3.450	3.000	2.370	2.550	2.100	0.000
LIP	0.000	0.000	0.000	0.000	0.000	0.000	3.900	3.450	3.000	2.370	2.550	2.100	0.000
CELL	0.000	0.000	0.000	0.000	0.000	0.000	3.900	3.450	3.000	2.370	2.550	2.100	0.000
WATER	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.030

Table A.11: Probability associated with different ingredient prices

Ingredient	Price (€/kg)	probability
LAS	0.105	0.3
	0.135	0.4
	0.18	0.3
AE+AA	0.135	0.3
	0.165	0.4
	0.21	0.3
MTEA	0.12	0.3
	0.15	0.4
	0.195	0.3
ZEOLITE + SILICONE	1.05	0.4
	1.35	0.3
	1.8	0.3
CMC	0.24	0.25
	0.3	0.35
	0.39	0.4
S.POLY	0.24	0.25
	0.3	0.35
	0.39	0.4
POLYGLY	0.24	0.25
	0.3	0.35
	0.39	0.4

Table A.12: Powd parameter (Martín & Martínez, 2018)

Ingredient	powd
LAS	0.115
AE	0.115
MTEA	0.115
STPP	0.111
Zeolite	0.111
Sodium perborate	0.125
Sodium percarbonate	0.125
Sodium sulfate	0.13
Xylene sulphonate	0.13
Antifoan	0.182
Protease	0.206
Lipase	0.206
Cellulose	0.206
Carboxymethyl cellulose	0.222
Sodium polyacrylate	0.222
Polietilen glicol	0.222
Water	0.111

Table A.13: Distance between the factory and suppliers (Google, 2019)

Supplier	Distance(km)
1	1539
2	685
3	533
4	674
5	857
6	973
7	70
8	222
9	378
10	525
11	427
12	760

Table A.14: Variable cost of pool (Martín & Martínez, 2018)

Tank	Cost parameter(€/Kg)
1	0.386
2	0.289
3	0.110
4	0.386
5	0.386

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B

APPENDIX B: SUPPLEMENTARY INFORMATION OF CHAPTER 4

Original model of Taifouris et al., 2020 adapted to 14 ingredients.
Mass balances and process constraints.

$$\sum_{sup,po} ccp_{ye,i,sup,po} = \sum_{l} x_{ye,i,l} + \sum_{j} z_{ye,i,j} \quad \forall ye, i \tag{B.1}$$

$$\sum_{sup} Lsup_{i,sup} = Au_i \quad \forall i \tag{B.2}$$

$$\sum_{sup} Linf_{i,sup} = Al_i \quad \forall i \tag{B.3}$$

$$Linf_{i,sup} < \sum_{po} ccp_{ye,i,sup,po} < \mathrm{Lsup}_{i,sup} \quad \forall ye,\ i \tag{B.4}$$

$$A_i^L \leq \sum_{l} x_{ye,i,l} + \sum_{j} z_{ye,i,l} \leq A_i^U \quad \forall ye, i \tag{B.5}$$

$$\sum_{l} x_{ye,i,l} \leq S_l \quad \forall\ ye, l \tag{B.6}$$

$$D_{ye,j}^L \ \leq \sum_{l} y_{ye,l,j} + \sum_{i} z_{ye,i,j} \leq D_{ye,j}^U \quad \forall ye, j \tag{B.7}$$

$$\sum_{i}^{14} x_{ye,i,l} = \sum_{j}^{3} y_{ye,l,j} \quad \forall ye, l \tag{B.8}$$

$$\sum_{i}^{14} CC_{i,k} \cdot x_{ye,i,l} = \sum_{j}^{3} p_{ye,l,k} \cdot y_{ye,l,j} \quad \forall\ \mathrm{ye, l, k} \tag{B.9}$$

$$P_{j,1}^{L} \leq \left(PQ_{j,1} + PQ_{j,2}\right) \quad \leq P_{j,1}^{G} \quad \forall j \tag{B.10}$$

$$P_{j,2}^{L} \leq \left(PQ_{j,3} + PQ_{j,4}\right) \quad \leq \ P_{j,2}^{G} \quad \forall j \tag{B.11}$$

$$P_{j,3}^{L} \leq \left(PQ_{j,5} + PQ_{j,6}\right) \leq P_{j,3}^{G} \quad \forall j \tag{B.12}$$

$$P_{j,4}^{L} \leq \left(PQ_{j,7} + PQ_{j,8}\right) \quad \leq P_{j,4}^{G} \quad \forall j \tag{B.13}$$

$$P_{j,5}^{L} \leq PQ_{j,9} \quad \leq \ P_{j,5}^{G} \quad \forall j \tag{B.14}$$

$$P_{j,6}^{L} \leq \left(PQ_{j,10} + PQ_{j,11}\right) \quad \leq \ P_{j,6}^{G} \quad \forall j \tag{B.15}$$

$$P_{j,7}^{L} \leq \left(PQ_{j,12} + PQ_{j,13}\right) \leq \ P_{j,7}^{G} \quad \forall j \tag{B.16}$$

$$P_{j,8}^{L} \leq \left(PQ_{j,14}\right) \leq \quad P_{j,8}^{G} \quad \forall j \tag{B.17}$$

$$PQ_{j,k} \cdot \left(\sum_{l} y_{ye,l,j} + \sum_{i} z_{ye,i,j}\right) = \sum_{i} CC_{i,k} \cdot z_{ye,i,j} + \sum_{l} p_{ye,l,k} \cdot y_{ye,l,j} \quad \forall ye, j, k \tag{B.18}$$

$$0 \leq x_{ye,i,l} \leq min \left\{ A_{i}^{U}, S_{l}, \sum_{j} D_{ye,j}^{U} \right\} \quad \forall ye, i, l \tag{B.19}$$

$$0 \leq y_{ye,l,j} \leq min \left\{ S_{l}, D_{ye,j}^{U}, \sum_{i} A_{i}^{U} \right\} \quad \forall ye, l, j \tag{B.20}$$

$$0 \leq z_{ye,i,j} \leq min\left\{D^U_{ye,j}, A^U_i\right\} \quad \forall ye, i, j \tag{B.21}$$

$$0 \leq p_{ye,l,k}, \leq max\left\{CC\left(i,k\right)\right\} \qquad \forall ye, i, j \tag{B.22}$$

Calculation of product performance

$$Performance_j = (107 \cdot \left(PQ_{j,surf1} + PQ_{j,surf2}\right) + 1872 \cdot \left(PQ_{j,enz1} + PQ_{j,enz2}\right) + 53.9 \cdot \left(PQ_{j,bu1} + PQ_{j,bu2}\right) + 134 \cdot \left(PQ_{j,pol1} + PQ_{j,pol2}\right) + 119 \cdot \left(PQ_{j,bl1} + PQ_{j,bl2}\right) \quad \forall j \tag{B.23}$$

And it is necessary that:
0.95 $\geq$ (High quality and high price) $\geq$ 1
0.8 $\geq$ (Average quality and average price) $\geq$ 0.95
0.7 $\geq$ (Average quality and average price) $\geq$ 0.80

Process constraints

$$Particle_j = 224.5 + 1509.78 \cdot PQ_{j,water} + 1000 \cdot \left(PQ_{j,filler1} + PQ_{j,filler2}\right) - 31 \cdot PQ_{j,water} \cdot \left(PQ_{j,filler1} + PQ_{j,filler2}\right) \qquad \forall j \tag{B.24}$$

Where Particle:

$$400\mu\text{m} < Particle_j < 500\mu\text{m} \quad \forall j \tag{B.25}$$

$$Cakest_j = 2.98 \cdot PQ_{j,water} + 2.69 \cdot \left(PQ_{j,poly1} + PQ_{j,poly2}\right) + 0.08 \cdot PQ_{j,water} \cdot \left(PQ_{j,poly1} + PQ_{j,poly2}\right) \quad \forall j \tag{B.26}$$

Where Cakest:

$$Cakest_j < 1kg \forall j \tag{B.27}$$

Calculation of ingredients and transportation cost. Price policies.

$$costj_{ye,i,sup,1} = c0_{i,prov} - \left(\frac{c0_{i,sup} \cdot discount}{Lsup_{i,sup} - Linf_{i,sup}}\right) \cdot \left(ccp_{ye,i,sup,1} - Linf_{i,sup}\right)$$

$\forall ye, i, sup$

$$(B.28)$$

$$costj_{ye,i,sup,2} = c0_{i,sup} \cdot \left(\frac{1}{1+disct}\right) + c0_{i,sup} \cdot \left(\frac{\left(\exp\left(-\left(\left(\frac{1}{Lsup_{i,sup}}\right)+\left(\frac{10}{Lsup_{i,sup}}\right)\cdot ccp_{ye,i,sup,2}\right)\right)\right)}{\left(\text{disct}+\exp\left(-\left(\left(\frac{1}{Lsup_{i,sup}}\right)+\left(\frac{10}{Lsup_{i,sup}}\right)\cdot ccp_{ye,i,sup,2}\right)\right)\ \right)}\right) \quad \forall \text{ye}, \text{i}, \text{sup} \tag{B.29}$$

$$costj_{ye,i,sup,3} = c0_{i,sup} \cdot \left(ccp_{ye,i,\text{sup},3}\right)^{\left(-powd_{i,\text{sup}}\right)} \qquad \forall ye, i, sup \tag{B.30}$$

$$costj_{ye,i,sup,4} = c0_{i,sup} \cdot (1 - fixdisc) \qquad \forall ye, i, sup \tag{B.31}$$

Total cost of the ingredients with price policies

$$cost_{ye,i,sup} = \sum_{po} costj_{ye,i,sup,po} \qquad \forall ye, i, sup \tag{B.32}$$

Total cost of the ingredients

$$CostP_{ye,i,sup} = cost_{ye,i,sup} + Costf_i \forall ye, i, \text{sup} \tag{B.33}$$

Transportation cost

$$Ctrans_{sup} = distance_{sup} \cdot priceT \qquad \forall sup \tag{B.34}$$

$$CTransU_{sup} = \frac{Ctrans_{sup}}{Loading\ capacity} \qquad \forall sup \tag{B.35}$$

$$CTT_{sup} = CtransU_{sup} \cdot \sum_{i,ye} ccp_{ye,i,sup} \qquad \forall sup \tag{B.36}$$

$$CTTT = \sum_{sup} CTT_{sup} \tag{B.37}$$

Main objective function

$$Beneficios = \sum_{ye,l,j} priceprod_j \cdot y_{ye,l,j} + \sum_{ye,i,j} priceprod_j \cdot z_{ye,i,j} - \sum_{ye,i,sup,po} CostP_{ye,i,sup,po} \cdot ccp_{ye,i,sup,po} - \ CTTT - \ \sum_{l} c\_pool_l \cdot \sum_{ye,l,j} y_{ye,l,j} \tag{B.38}$$

Penalties

$$\text{penalty}_{1,i,sup,po} = \sum_{po} ccp_{1,i,sup,po} - \text{ccp}_{1,\text{i},\text{sup},\text{po}} \forall i, \text{sup}, \text{po} \tag{B.39}$$

$$\text{penalty}_{2,i,sup,po} = \sum_{po} \sum_{sup} ccp_{1,i,sup,po} + \sum_{po} ccp_{2,i,sup,po} - \text{ccp}_{1,\text{i},\text{sup},\text{po}} - \text{ccp}_{2,\text{i},\text{sup},\text{po}} \quad \forall i, \text{sup}, \text{po} \tag{B.40}$$

Information about of case of study We set the discount parameters of the different policies with the following values:

- Discount = **0.5**
- Disct = **1**
- Fixdisc = **0.15**

The tables B.1-B.12, which are used in the case of study and they were not included in the manuscript, are attached below:

Table B.1: Maximum available amount of the raw material (Martín & Martínez, 2018)

Supplier/Ingredient(t)	Inorganic			Organic			Enzyme			Water
LAS	0	0	0	400	400	400	0	0	0	0
AE	0	0	0	400	400	400	0	0	0	0
STPP	500	500	500	0	0	0	0	0	0	0
Zeolite	500	500	500	0	0	0	0	0	0	0
Sodium perborate	250	250	250	0	0	0	0	0	0	0
Sodium percarbonate	250	250	250	0	0	0	0	0	0	0
Sodium sulfate	200	200	200	0	0	0	0	0	0	0
Xylene sulphonate	200	200	200	0	0	0	0	0	0	0
Antifoan	0	0	0	50	50	50	0	0	0	0
Protease	0	0	0	0	0	0	30	30	30	0
Lipase	0	0	0	0	0	0	30	30	30	0
Sodium polyacrylate	0	0	0	20	20	20	0	0	0	0
Polietilen glicol	0	0	0	20	20	20	0	0	0	0
Water	0	0	0	0	0	0	0	0	0	500

Table B.2: Size of the intermediate tanks (Martín & Martínez, 2018)

Tank	**Size (m^3)**
1	300.5
2	300.5
3	300.5
4	300.5
5	300.5

Table B.3: Variable cost of pool (Martín & Martínez, 2018)

Tank	Cost parameter(€/kg)
1	0.386
2	0.289
3	0.110
4	0.386
5	0.386

Table B.4: Composition of ingredient k in the flow (Martín & Martínez, 2018)

t_i/t_k	1	2	3	4	5	6	7	8	9	10	11	12	13	14
LAS	1	0	0	0	0	0	0	0	0	0	0	0	0	0
AE	0	1	0	0	0	0	0	0	0	0	0	0	0	0
STPP M1	0	0	1	0	0	0	0	0	0	0	0	0	0	0
Zeolite	0	0	0	1	0	0	0	0	0	0	0	0	0	0
Sodium perborate	0	0	0	0	1	0	0	0	0	0	0	0	0	0
Sodium percarbonate	0	0	0	0	0	1	0	0	0	0	0	0	0	0
Sodium sulfate	0	0	0	0	0	0	1	0	0	0	0	0	0	0
Xylene sulphonate	0	0	0	0	0	0	0	1	0	0	0	0	0	0
Antifoan	0	0	0	0	0	0	0	0	1	0	0	0	0	0
Lipase	0	0	0	0	0	0	0	0	0	1	0	0	0	0
Cellulose	0	0	0	0	0	0	0	0	0	0	1	0	0	0
Sodium polyacrylate	0	0	0	0	0	0	0	0	0	0	0	1	0	0
Polietilen glicol	0	0	0	0	0	0	0	0	0	0	0	0	1	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Table B.5: Maximum concentration of the group of ingredients g in the product j (Martín & Martínez, 2018)

t_i/t_j	1	2	3	4	5	6	7	8
1	0.250	0.600	0.250	0.500	0.050	0.050	0.050	0.500
2	0.250	0.600	0.250	0.500	0.050	0.010	0.050	0.500
3	0.250	0.600	0.250	0.600	0.050	0.010	0.050	0.500

Table B.6: Minimum concentration of the group of ingredients g in the product j (Martín & Martínez, 2018)

t_i/t_j	1	2	3	4	5	6	7	8
1	0.150	0.100	0.050	0.100	0.001	0.001	0.001	0.005
2	0.150	0.100	0.050	0.100	0.001	0.001	0.001	0.005
3	0.150	0.100	0.050	0.100	0.001	0.001	0.001	0.005

Table B.7: Prices without discounts

Ingredient	**Price(€/kg)**
STPP	0.048
ZE	0.030
S. PERBO	0.300
S. PERCA	0.300
S.SU	0.030
X.SU	0.060
LIP	2.550
CELL	2.550
WATER	0.030

Table B.8: Probability associated with different ingredient prices

Ingredient	Price (€/kg)	probability
LAS	0.105	0.3
	0.135	0.4
	0.18	0.3
AE+AA	0.135	0.3
	0.165	0.4
	0.21	0.3
MTEA	0.12	0.3
	0.15	0.4
	0.195	0.3
ZEOLITE + SILICONE	1.05	0.4
	1.35	0.3
	1.8	0.3
CMC	0.24	0.25
	0.3	0.35
	0.39	0.4
S. POLY	0.24	0.25
	0.3	0.35
	0.39	0.4
POLYGLY	0.24	0.25
	0.3	0.35
	0.39	0.4

Table B.9: Powd parameter (Martín & Martínez, 2018)

Ingredient	**powd**
LAS	0.115
AE	0.115
MTEA	0.115
STPP M1	0.111
Zeolite	0.111
Sodium perborate	0.125
Sodium percarbonate	0.125
Sodium sulfate	0.13
Xylene sulphonate	0.13
Antifoan	0.182
Protease	0.206
Lipase	0.206
Cellulose	0.206
Carboxymethyl cellulose	0.222
Sodium polyacrylate	0.222
Polietilen glicol	0.222
Water	0.111

Table B.10: Coordinate of locations

Location	Latitude	Longitudes
1	38.6514145	-6.3272768
2	40.5974808	-6.0855775
3	43.213385	-6.1185365
4	38.6685722	-3.9981752
5	40.6475136	-3.6356264
6	43.3733134	-3.756476
7	38.6762147	-1.3091006
8	40.6466051	-1.1772647
9	43.1519603	-1.0783877
10	41.3366954	1.780065
11	42.7237694	1.7800097
12	45.4353833	1.4956473
13	47.7452074	1.5414098
14	49.5046875	1.3842991
15	51.2694508	0.585748
16	43.531953	3.7840965
17	45.4910965	3.6082255
18	47.7691761	3.6088434
19	49.52648	3.6518218
20	50.7931951	3.6304176
21	43.5661627	5.6952564
22	45.5220087	5.651557
23	47.7983612	5.6082125
24	49.5671274	5.6736232
25	51.0546287	5.607827
26	52.2292051	5.5205179
27	43.9130601	7.9369286
28	45.6597198	7.8050084
29	47.7836195	7.7611473

Table B.11: Coordinates of suppliers

Supplier	Latitude	Longitudes
1	41.1403127	-8.5805843
2	43.3904082	-5.6093616
3	42.003318	-1.5491137
4	39.2701482	-0.4174544
5	41.4045401	2.0322086
6	43.5695249	1.8483396
7	46.0958652	1.472194
8	47.7587867	-2.1287112
9	49.0631074	2.7045579
10	49.3620004	3.416486
11	49.1468772	7.5473453
12	46.2256265	5.0752702
13	51.5584845	5.0883731
14	45.778667	4.8120378
15	45.3214308	7.7779069
16	45.6402267	12.5146265
17	47.4812184	9.5908024
18	49.7253323	9.1972277
19	45.0822104	11.5702746
20	49.4946927	8.4323656
21	52.3422738	9.5529255
22	51.2093574	6.786942
23	45.2541877	8.7395574
24	50.0977486	14.4121417
25	48.1987693	16.257549
26	45.8376188	16.2265446
27	48.5538517	17.678673
28	51.7849916	19.4962266
29	50.439376	20.9301538
30	49.4535146	7.6515266
31	51.1030488	7.5937823

32	52.3818457	7.3081378
33	53.4287249	7.2641924
34	43.8571701	10.6040362
35	45.881273	10.3843096
36	47.7758558	9.8790131
37	49.4318831	9.7689859
38	51.086436	9.5488916
39	52.3260637	9.5269127
40	53.4780553	9.4394517
41	43.8096436	12.9551104
42	45.8818014	12.7351667
43	47.8094442	12.5600997
44	49.4503241	12.3626204
45	51.1069152	12.2521156
46	52.4856695	12.0762042
47	53.5306794	11.9661254
48	41.6307242	14.9985674
49	45.5591471	14.9765948
50	47.7910448	14.888182
51	49.4525746	14.8499825
52	51.1511142	14.7403315
53	52.429388	14.6740787
54	44.0702974	18.2965094
55	47.9885215	17.9010016
56	49.7089198	17.8790289
57	51.1652371	17.6376887
58	52.4824815	17.5049954
59	54.469172	17.3768905
60	48.0307133	20.9343945
61	49.8147533	20.9084317
62	51.2666893	20.8414321
63	52.6950932	20.7574469
64	54.4823691	20.6469151

65	49.8356388	23.1496562
66	51.3152038	22.9298118
67	52.7472547	23.0398395
68	54.4828703	23.0639132

Table B.12: Coordinates of customers

Customers	Latitude	Longitudes
1	-3.6904614	40.389787
2	-2.5698559	37.2230337
3	-2.4160473	43.1744664
4	-3.4487622	40.7569621
5	6.4926118	43.4557732
6	2.3773842	49.5898921
7	-9.1735741	38.8675817
8	16.332492	48.1198406
9	4.2216534	50.7323422
10	7.8166513	51.6796986
11	6.2993782	47.6873359
12	10.7444452	43.6877656
13	20.5589886	51.9730926
14	26.0037154	44.9239604

Table B.13: Nomenclature

Al_i	Minimum amount of raw material necessary for the process (t)
Au_i	Maximum amount of raw material i supported by the process (t)
C_{pool}	Variable cost of pool l(€/kg)
$Co_{i,sup}$	Price without discount of raw material i of supplier sup(€/kg)
capacity	Loading capacity (kg)
$CC_{i,k}$	Composition of ingredient k in the flow I (ti/tk)
$Costf_{s,i}$	Average price of the ingredient price with uncertainty (€/kg)
$Costh_i$	High value of the ingredient price with uncertainty(€/kg)
$Costjf_{s,i}$	Ingredient cost with uncertainty i in the scenario s (€/kg)
$Costl_i$	Low value of the ingredient price with uncertainty(€/kg)
$Costm_i$	Medium value of the ingredient price with uncertainty(€/kg)
Discount	Discount parameter of policy 1
Disct	Discount parameter of policy 2
Distancesup	Distance from the supplier sup to the manufacturer(km)
$DL_{ye,j}$	Minimum demand in the year ye of the product j(t)
$DU_{ye,j}$	Maximum demand in the year ye of the product j(t)
Fixdisc	Discount parameter of policy 4
Linf $_{i,sup}$	Minimum amount of the flow i by the sup supplier (t)
$Lsup_{i,sup}$	Maximum available amount of the flow i by the sup supplier (t)
$PG_{j,g}$	Maximum concentration of the group of ingredients g in the product j(ti/tj)
$PL_{j,g}$	Minimum concentration of the group of ingredients g in the product j (ti/tj)
$Powd_i$	Discount parameter of policy 3
PriceT	Transport price (€/km)
Proh	Probability of high price
Prol	Probability of low price
Prom	Probability of medium price
S_l	Maximum tank size (t)
$Priceprod_j$	Price of the product j (€/kg)
Variables	
$Cakest_j$	Cake size of the product j
$ccp_{ye,i,sup,po}$	Amount purchased from ingredient i to supplier sup using policy po and in year ye (ti/year)
$costj_{ye,i,sup,po}$	Raw material i cost applying the discount of the policy po of the supplier sup the year ye
$CostP_{ye,i,sup,po}$	Combined cost of the ingredients fixed by contract and with uncertainty
$Cost_{ye,i,sup,po}$	
$Ctrans_{sup}$	Cost of transport(€/km)
$CTransU_{sup}$	Unit cost of transport for the supplier sup
CTT_{sup}	Total transport cost of the supplier sup
CTTT	Total transport cost
$MassProd_{ye,j}$	Amount produced of product j per year
$Particle_j$	Particle size of the product j (µm)
$penalty_{ye,i,sup,po}$	Penalty for supplier or policy repetition
$Performance_j$	Performance of product (j)
$PQ_{j,k}$	Composition in component (k) of product (J)
profit	Profit obtained
$p_{ye,l,k}$	Composition in component (k) of pool (l)
$x_{ye,i,l}$	Flows from raw material (i) to intermediate pool(l) (ti/year)
$y_{ye,l,j}$	Flow from pool (l) to product (j) (ti/year)
$z_{ye,i,j}$	Flow from raw material (i) to product (j) (ti/year)
Subscript	
g	Group of the ingredients
I	Stream of raw material
j	Product
k	Ingredient

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C

APPENDIX C: SUPPLEMENTARY INFORMATION OF CHAPTER 5

C.1 MODEL FOR ESTIMATING NUTRITIONAL AND ENERGY NEEDS OF CATTLE (COUNCIL, 2000)

C.1.1 *Energy and protein requirements for gain*

Firstly, the amount of weight the animal must gain before the first pregnancy must be determined (BPADG$_t$). Eq.(C.1) is used to estimate this amount, where TPW is the weight the animal should have when it becomes pregnant, TAGE$_t$ is the age of the animal, TPA is the age at which it becomes pregnant and SBW$_t$ is Shrunk body weight (96% of the real weight of the animal). 't' is the temporal set formed by 72 time periods of 24 days. The SBW$_t$ is calculated with the body weight (BW$_t$) using Eq.(C.2). The body weigh BW$_t$ in the period time 't' is updated with the body weight of previous period time BW$_{t-1}$ and BPADG$_t$(Eq.(C.3)).

$$\text{BPADG}_\text{t}\text{(kg/day)=}\frac{\text{TPW(kg)-SBW}_\text{t}\text{(kg)}}{\text{TPA(day)-TAGE}_\text{t}\text{(day)}}\ \forall t \tag{C.1}$$

$$\text{SBW}_\text{t}\text{=0.96}\cdot\text{BW}_\text{t}\ \forall t \tag{C.2}$$

$$\text{BW}_\text{t}\text{=BW}_\text{t-1}\text{+BPADG}_\text{t}\text{(kg/day)}\quad \forall t \tag{C.3}$$

The TPW is 55% of the mature weight of the animal (MW) and the TPA is 440 days. Therefore, the daily amount of gain (SWG$_t$) is equal to the BPADG$_t$ for the first pregnancy. The daily gain during pregnancy (APADG$_t$) is given by Eq.(C.4).

$$\text{APADG}_\text{t}\text{(kg/day)=}\frac{\text{TCW}_1\text{(kg)-TPW(kg)}}{\text{280days}}\ \forall t \tag{C.4}$$

Where TCW1 is the target weight after calving of the first calf (80% of MW). After the first calving, the daily growth between calves (ACADG$_t$) will be given by Eq.(C.5).

$$\text{ACADG}_\text{t}\text{(kg/day)=}\frac{\text{TCW}_\text{xx}\text{(kg)-TCW}_\text{x}\text{(kg)}}{\text{CI(day)}}\ \forall t \tag{C.5}$$

Where the objective weights of the second and third calving are 92% and 96% of the MW respectively. Each cow will only be considered to have 3 calving before being slaughtered for meat production. Therefore, depending on the period of the animal, the necessary daily growth will be different:

- SWG = BPADG before the first calving.
- SWG = APADG during the first calving.
- SWG = ACADG among the rest of the deliveries.

The RE_t needed to reach those weights will be given by Eq.(C.6).

$$\mathrm{RE_t(Mcal/day)}=0.0635\cdot \mathrm{EQEBW_t(kg)}\cdot 0.75\cdot \mathrm{EBG_t(kg)}\cdot 1.097\ \forall t \tag{C.6}$$

Where $EQEBW_t$ is the equivalent empty body weight and is calculated by Eq.(C.7).

$$\mathrm{EQEBW_t(kg)}=0.891\cdot \mathrm{EQSBW_t(kg)}-\frac{\mathrm{ADGpreg_t(g)}}{1000}\ \forall t \tag{C.7}$$

Where $EQSBW_t$ is equivalent shrunk body weight and is calculated by Eq.(C.8).

$$\mathrm{EQSBW_t(kg)}=\mathrm{SBW_t(kg)}\cdot\left(\frac{\mathrm{SRW}_t\mathrm{(kg)}}{\mathrm{FSBW(kg)}}\right)\ \forall t \tag{C.8}$$

Where SRW_t is a reference weight based on the final fat that the animal may have and FSBW is final shrunk body weight at the expected final body fat. Whereas $ADGpreg_t$ is the daily weight gain due to pregnancy and is calculated by Eq.(C.9), where t is the day of pregnancy.

$$\begin{aligned}&\mathrm{ADGpreg_t(g)}=\mathrm{CBW(kg)}\cdot(18.28\cdot(0.02\text{-}0.0000286\cdot \mathrm{tpreg_t(day)})\cdot\\&e^{(0.02\cdot \mathrm{tpreg_t(day)}-0.0000143\cdot \mathrm{tpreg_t(day)}^2)})\ \forall t\end{aligned} \tag{C.9}$$

EBG_t is the daily gain assuming the body is empty and is estimated by Eq.(C.10).

$$\mathrm{EBG_t(kg)}=0.956\cdot \mathrm{SWG_t(kg)}\ \forall t \tag{C.10}$$

On the other hand, the estimation of the proteins necessary for growth (NPg_t) is given by Eq.(C.11), while the necessary metabolizable protein (MPg_t) depends on the value of $EQEBW_t$. If its value is below 300kg, Eq.(C.12) is applied otherwise, Eq.(C.13) is applied. Due to the weight can be correlated with the time, Eq.(C.12) will be used for an age (in weeks) less than 57 and Eq.(C.13) for an age greater than 57. EBG_t is related to RE_t as indicated in Eq.(C.14).

$$\mathrm{NPg_t(g/day)=SWG_t(kg)\cdot(296\text{-}(29.4(RE_t(Mcal/day)/SWG_t(kg))))}\ \forall t \tag{C.11}$$

$$\mathrm{MPg_t(g/day)=\frac{NPg_t(g/day)}{0.834\text{-}(EQSBW_t(kg)\cdot 0.00114)}}\forall t \tag{C.12}$$

$$\mathrm{MPg_t(g/day)=\frac{NPg_t(g/day)}{0.492}}\forall t \tag{C.13}$$

$$\mathrm{EBG_t(kg)=12.341\cdot EQEBW_t(kg)^{-0.6837}\cdot RE_t(Mcal/day)^{0.9116}}\ \forall t \tag{C.14}$$

C.1.2 *Total maintenance energy and protein requirement*

The energy required to meet the basal needs of cattle (NEm_t) is calculated using Eq.(C.15) and is influenced by temperature (TP), breed (BE), if it is a lactating (L = 1.2) or not (L = 1) or the nutrition plan (COMP) which is calculated by Eq.(C.16) and dependency condition score (CS) on a scale of 1 to 9 (it is considered a value of 5). In this work, since a particular location is not specified, the value of Be is considered to be 1.

$$\begin{aligned}&\mathrm{NEm_t(Mcal/day)=SBW_t(kg)^{0.75}\cdot((0.077(Mcal/day\cdot kg^{0.75})\cdot BE\cdot L\cdot COMP)}\\&\mathrm{+0.0007(Mcal/(day\cdot kg^{0.75}\ {}^{o}C))\cdot(20\text{-}T_P))}\ \forall t\end{aligned} \tag{C.15}$$

$$\mathrm{COMP=0.8+((CS\text{-}1)\cdot 0.05)}\ \forall t \tag{C.16}$$

If the cow is pregnant, it will be necessary to add an extra metabolic energy ($NEmpreg_t$), which is indicated by Eq.(C.17) . Where CBW represents the calf birth weight and the value that has been used has been 31 kg, and km is the value for efficiency of utilization of energy for maintenance and its value is 0.576.

$$\begin{aligned}&\mathrm{NEmpreg_t(Mcal/day)=CBW(kg)\cdot\left(\frac{k_m}{0.13}\right)\cdot}\\&\mathrm{(0.05855\text{-}0.0000996\cdot tpreg_t(day))\cdot e^{(0.03233\text{-}0.0000275\cdot tpreg_t(day))\cdot tpreg_r(day))}}\\&\forall t\end{aligned} \tag{C.17}$$

The amount of food that cattle must eat to supply maintenance energy (Im_t) is calculated by Eq.(C.18) and depends on the maintenance energy (NEm_t), the energy of the maintenance diet ($Nema_t$) and if that diet contains ionophores (ADTV = 1.12) otherwise (ADTV 1.0)

$$\mathrm{Im_t(kg/day)}=\frac{\mathrm{NEm_t(Mcal/day)}}{\mathrm{NEma_t(Mcal/kg)\cdot ADTV}}\ \forall t \tag{C.18}$$

The $Nema_t$ is calculated using the formulation of the diet, $x_{j,t}$ (Eq.(C.19)), where $Nemac_j$ is the Nema of each crop.

$$\mathrm{Nema_t}=\sum_j \mathrm{x_{t,j}}\cdot \mathrm{Nemac_j}\ \forall t \tag{C.19}$$

The energy available for livestock growth (RE_t) is estimated by Eq.(C.20) , where DMI_t is the total amount of dry food ingested by the animals and $NEga_t$ is the amount of energy from the diet invested in the growth of the animal.

$$\mathrm{RE_t(Mcal/day)=(DMI_t(kg/day)\text{-}Im_t(kg/day))\cdot NEga_t(Mcal/day)}\ \forall t \tag{C.20}$$

The $Nega_t$ is calculated using the formulation of the diet and the Eq.(C.21), where $Negac_j$ is the Nega of each crop.

$$\mathrm{Nega_t}=\sum_j \mathrm{x_{t,j}}\cdot \mathrm{Negac_j}\ \forall t \tag{C.21}$$

The amount of daily feed eaten by cattle depends on their growth stage. On the one hand, for calves and yearlings, the amount ingested is given by Eqs.C.22 and C.23 where there are a series of corrections for due to the presence of anabolic stimulant in food (ADTV=1.0, otherwise ADTV=0.94), for temperature (TEMP1), for their hair size (MUD1), for body fat (BFAF) and breed (BI). For this work, it will be considered that cattle live in a region with a temperature range from 5 to 15 degrees (TEMP1 = 1.03), they will have a hair size of less than 10 cm (Mud1 = 1), a medium body fat (BFAF = 0.90) and a breed other than Holstein (Bi = 1).

$$\mathrm{DMI_t(kg/day)}=\left(\frac{\mathrm{SBW_t(kg)^{0.75}\cdot(0.2435\cdot NEma_t(Mcal/day)\text{-}0.0466\cdot NEma_t(Mcal/day)^2\text{-}0.1128))}}{\mathrm{NEma_t(Mcal/day)}}\right)\cdot$$
$$\mathrm{BFAF\cdot BI\cdot ADTV\cdot TEMP1\cdot MUDI}\ \forall t \tag{C.22}$$

$$\mathrm{DMI_t(kg/day)}=\left(\frac{\mathrm{SBW_t(kg)^{0.75}\cdot(0.2435\cdot NEma_t(Mcal/day)\text{-}0.0466\cdot NEma_t(Mcal/day)^2\text{-}0.0869))}}{\mathrm{NEma_t(Mcal/day)}}\right)\cdot$$
$$\mathrm{BFAF\cdot BI\cdot ADTV\cdot TEMP1\cdot MUDI}\ \forall t$$

(C.23)

On the other hand, for non-pregnant lactating cows and pregnant lactating cows, the amount of feed ingested will be given by Eqs.C.24-C.25. The daily milk production factor (Yn) is to be added to these equations.

$$DMI_t(kg/day)=\left(\frac{SBW_t(kg)^{0.75}\cdot(0.04997\cdot NEma_t{}^2(Mcal/day)+0.03840)}{NEma_t(Mcal/day)}\right)\cdot TEMP1\cdot (MUDI+0.2\cdot Yn)\forall t \tag{C.24}$$

$$DMI_t(kg/day)=\left(\frac{SBW_t(kg)^{0.75}\cdot(0.04997\cdot NEma_t{}^2(Mcal/day)+0.04631)}{NEma_t(Mcal/day)}\right)\cdot TEMP1\cdot (MUDI+0.2\cdot Yn)\forall t \tag{C.25}$$

The milk production factor is calculated by Eq.(C.26) where n is the week of lactation and 'k' and 'a' are given by Eqs.(C.27) and (C.28), respectively.

$$Yn_t(kg/day)=\frac{n}{a\cdot e^{kn}}\ \forall t \tag{C.26}$$

$$k=\frac{1}{T} \tag{C.27}$$

$$a=\frac{1}{PKYD(kg/day)\cdot k\cdot e} \tag{C.28}$$

The amount of milk produced must be corrected in the event that the cow is pregnant. The decrease in milk production (Ypn_t), which depends on the day of pregnancy (t) within the 280-day gestation cycle, is estimated by the correlation shown in Eq.(C.29).

$$Ypn_t(g/day)=((CBW(kg)\cdot(0.001669)\cdot (0.000000211\cdot tpreg_t(day))\cdot e^{(0.0279-0.0000176\cdot tpreg_t(day))\cdot tpreg_t(day))}))\cdot 6.25\forall t \tag{C.29}$$

The amount of proteins necessary for basal vital functions ($MPmain_t$) is estimated by Eq.(C.30).

$$MPmain_t(g/day)=3.8\cdot SBW_t(kg)^{0.75}\ \forall t \tag{C.30}$$

If the cow is pregnant, protein supplement ($MPpreg_t$) is required and computed by Eq.(C.31) .

$$MPpreg_t(g/day)=\frac{Ypn_t(g/day)}{0.65}\ \forall t \tag{C.31}$$

C.1.3 *Energy and protein reserves*

In Eqs C.32-C.35, the energy and nutritional reserves are indicated in the form of a proportion of fat (AF), protein (AP), water (AW) and ashes (AA).

$$\mathrm{AF}(\%\mathrm{EBW}){=}0.037683 \cdot \mathrm{CS} \tag{C.32}$$

$$\mathrm{AP}(\%\mathrm{EBW}){=}0.200886{-}0.0066762 \tag{C.33}$$

$$\mathrm{AW}(\%\mathrm{EBW}){=}0.766637{-}0.034506 \cdot \mathrm{CS} \tag{C.34}$$

$$\mathrm{AA}(\%\mathrm{EBW}){=}0.078982{-}0.034506 \cdot \mathrm{CS} \tag{C.35}$$

C.1.4 *Supply of nutrients and estimation of waste production*

Protein supplement

There are two sources of protein intake, the proteins from food ($\mathrm{MPFeed}_{t,j}$) and the protein from bacterial activity ($\mathrm{MPBact}_{t,j}$). Out of the protein available in food (UIP), 80% is digestible, and the contribution can be calculated from the nutritional information of the diet (Eq.(C.36)). To estimate the microbial contribution, the microbial crude protein yield ($\mathrm{MCP}_{t,j}$) is used, which is calculated from the total digestible nutrients and the percentage of degradability of the neutral detergent fiber of the diet (eNDF) using Eq.(C.37) . 64% is assumed to be true digestible protein (Eq.(C.38)). The total supplement will be the sum of the two contributions (Eq.(C.39)).

$$\begin{gathered}\mathrm{MPfeed}_{\mathrm{t,j}}(\mathrm{g/day}){=}\frac{\mathrm{UIP}(\%\mathrm{CP})}{100} \cdot \frac{\mathrm{CP}(\%\mathrm{DM})}{100} \cdot 0.8 \cdot \\ \mathrm{DMI}_{\mathrm{t}}(\mathrm{kg/day}) \cdot 1000\mathrm{g/kg} \cdot \mathrm{x}_{\mathrm{t,j}} \ \forall t, j\end{gathered} \tag{C.36}$$

$$\mathrm{MPC}_{\mathrm{t,j}}(\mathrm{g/day}){=}0.13 \cdot \mathrm{TDN}(\mathrm{g/day})/100 \cdot \mathrm{DMI}_{\mathrm{t}} \cdot \mathrm{x}_{\mathrm{t,j}} \ \forall t, j \tag{C.37}$$

$$\mathrm{MPBact}_{\mathrm{t,j}}(\mathrm{g/day}){=}\mathrm{MCP}_{\mathrm{t}}(\mathrm{g/day}) \cdot 0.64 \ \forall t, j \tag{C.38}$$

$$\mathrm{MPtot_{t,j}(g/day)}=\mathrm{MPbact_{t}(g/day)}+\mathrm{MPfeed_{t}(g/day)}\ \forall t,j \tag{C.39}$$

Supply of energy and protein

The total supply of carbohydrates (CHO_j), as well as the different types of carbohydrates, such as unavailable fiber (CC_j), available fiber ($CB2_j$), nonfiber carbohydrates (NFC_j), starch ($CB1_j$), sugar (CA_j) are estimated from nutritional information (crude protein (CP_j), neutral detergent fiber (NDF_j), lignin ($LIGNIN_j$), nonstructural carbohydrate ($STARCH_j$), neutral detergent insoluble protein in the crude protein ($NDFIP_j$), unavailable fiber (CC_j)) of the diet fed to the animals through Eqs.(C.40)-(C.45).

$$\mathrm{CHO_j(\%DM)}=100\text{-}\mathrm{CP_j(\%DM)}\text{-}\mathrm{FAT_j(\%DM)}\text{-}\mathrm{ASH_j(\%DM)}\ \forall j \tag{C.40}$$

$$\mathrm{CC_j(\%DM)}=\mathrm{NDF_j(\%DM)}\cdot 0.01\cdot \mathrm{LIGNIN_j(\%DM)}\cdot 2.4\ \forall j \tag{C.41}$$

$$\begin{aligned}&\mathrm{CB2_j(\%DM)}=\mathrm{NDF_j(\%DM)}\text{-}\\&(\mathrm{NDFIP_j(\%DM)}\cdot 0.01\cdot \mathrm{CP_j(\%DM)})\text{-}\mathrm{CC_j(\%DM)})\ \forall j\end{aligned} \tag{C.42}$$

$$\mathrm{NFC_j(\%DM)}=\mathrm{CHO_j(\%DM)}\text{-}\mathrm{CB2_j(\%DM)}\text{-}\mathrm{CC_j(\%DM)}\ \forall j \tag{C.43}$$

$$\mathrm{CB1_j(\%DM)}=\mathrm{STARCH_j(\%DM)}\cdot \mathrm{NDF_j(\%DM)}/100\ \forall j \tag{C.44}$$

$$\mathrm{CA_j(\%DM)}=\mathrm{NDF_j(\%DM)}\text{-}\mathrm{CB1_j(\%DM)}\ \forall j \tag{C.45}$$

Similarly, the different types of proteins supplied to animals are computed. 3 types of proteins are distinguished according to their degradation speed, $PB1_j$ (rapid), $PB2_j$ (intermediate) and $PB3_j$ (slow). To the above it is necessary to add the crude protein that is bound protein (PC_j). The calculation of the supply of these proteins is given by the nutritional information of the animals' diet (crude protein that is soluble protein ($SOLP_j$), crude protein that is non-protein nitrogen (PA_j), crude protein that is neutral detergent insoluble protein ($NDFIP_j$), crude protein that is acid detergent insoluble protein ($ADFI_j$)) through Eqs.(C.46)-(C.49).

$$\mathrm{PB1_j(\%DM)=SOLP_j(\%CP)\cdot CP_j\cdot 0.01\text{-}PA_j(\%DM)}\ \forall j \tag{C.46}$$

$$\mathrm{PB3_j(\%DM)=(NDFIP_j(\%CP)\text{-}ADFIP_j(\%CP))\cdot CP_j\cdot 0.01}\ \forall j \tag{C.47}$$

$$\begin{gathered}\mathrm{PB2_j(\%DM)=CP_j(\%DM)\text{-}PA_j(\%DM)\text{-}}\\ \mathrm{PB1_j(\%DM)\text{-}PB3_j(\%DM)\text{-}PC_j(\%DM)}\ \forall j\end{gathered} \tag{C.48}$$

$$\mathrm{PC_j(\%DM)=ADFIP_j(\%CP)\cdot CP_j(\%DM)\cdot 0.01}\ \forall j \tag{C.49}$$

Degradation of nutrients in the rumination phase

The amount of nutrient that is degraded and used during digestion in the rumination phase is given by the degradation ratio (Kp) that is estimated by Eq.(C.50) if it is forage and Eq.(C.51) if it is concentrate.

$$\mathrm{Kp[forage]=(0.388+(0.022\cdot DMI/SBW0.75)+2.0\cdot FORAGE2)/100} \tag{C.50}$$

$$\mathrm{Kp[conc]=\text{-}0.424+(1.45\cdot Kp[forage])} \tag{C.51}$$

While the non-degradation ratio (Kd) is specific to each food and each type of nutrient and is indicated in the nutritional information of the food itself. It is the total amount of component j of the DMI, which is calculated by Eq.(C.52) using the DMI_t and the fraction of component j in the DMI ($\mathrm{x}_{t,j}$). Using both ratios it is possible to determine the amount of each type of degraded (Eqs(.C.53)-(C.57)) and non-degraded (Eqs.(C.58)-(C.61)) proteins of each type. $\mathrm{RDPA}_{t,j}$, $\mathrm{RDPB1}_{t,j}$, $\mathrm{RDPB2}_{t,j}$, RDPB3 are the degraded amount of $\mathrm{PA}_{t,j}$, $\mathrm{PB1}_{t,j}$, $\mathrm{PB2}_{t,j}$, $\mathrm{PB3}_{t,j}$; and $\mathrm{REPB1}_{t,j}$, $\mathrm{REPB2}_{t,j}$, $\mathrm{RDPB3}_{t,j}$, $\mathrm{REPC}_{t,j}$ are the non-degraded amount.

$$\mathrm{It_{t,j}(g/day)=DMI_{\mathit{t}}(kg/day)\cdot x_{t,j}\cdot 1000g/kg}\ \forall t,j \tag{C.52}$$

$$\mathrm{RDPA_{t,j}=It_{t,j}\cdot PA_j}\ \forall t,j \tag{C.53}$$

$$\mathrm{RDPB1_{t,j}(g/day)=It_{t,j}(g/day)\cdot PB_{1j}}\cdot\left(\frac{\mathrm{Kd_{1j}}}{\mathrm{(Kd_{1j}+Kp_j}}\right)\ \forall t,j \tag{C.54}$$

$$\mathrm{RDPB2_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{PB_{2j}} \cdot \left(\frac{\mathrm{Kd_{2j}}}{\mathrm{Kd_{2j}{+}Kp_{j}}}\right) \; \forall t, j \tag{C.55}$$

$$\mathrm{RDPB3_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{PB_{3j}} \cdot \left(\frac{\mathrm{Kd_{3j}}}{\mathrm{Kd_{3j}{+}Kp_{j}}}\right) \; \forall t, j \tag{C.56}$$

$$\begin{aligned}&\mathrm{RDPEP_{t,j}(g/day){=}RDPB1_{t,j}(g/day){+}RDPB2_{t,j}(g/day)}\\&\mathrm{{+}RDPB3_{t,j}(g/day)} \; \forall t, j\end{aligned} \tag{C.57}$$

$$\mathrm{REPB1_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{PB_{1j}} \cdot \frac{\mathrm{Kp_{j}}}{\mathrm{Kd_{1j}{+}Kp_{j}}} \; \forall t, j \tag{C.58}$$

$$\mathrm{REPB2_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{PB_{2j}} \cdot \frac{\mathrm{Kp_{j}}}{\mathrm{Kd_{2j}{+}Kp_{j}}} \; \forall t, j \tag{C.59}$$

$$\mathrm{REPB3_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{PB_{3j}} \cdot \frac{\mathrm{Kp_{j}}}{\mathrm{Kd_{3j}{+}Kp_{j}}} \; \forall t, j \tag{C.60}$$

$$\mathrm{REPC_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{PC_{j}} \; \forall t, j \tag{C.61}$$

The carbohydrates are computed similarly. Eqs.(C.62)-(C.64) estimate the amount of degraded CA_j, $CB1_j$ and $CB2_j$ ($RDCA_{t,j}$, $RDCB1_{t,j}$ and $RDCB2_{t,j}$, respectively) and Eqs.(C.65)-(C.67) estimate the amount of non-degradation ($RECA_{t,j}$, $RECB1_{t,j}$ and $RECB2_{t,j}$).

$$\mathrm{RDCA_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{CA_{j}} \cdot \left(\frac{\mathrm{Kd_{4j}}}{\mathrm{Kd_{4j}{+}Kp_{j}}}\right) \; \forall t, j \tag{C.62}$$

$$\mathrm{RDCB1_{t,j}(g/day)_{j}{=}It_{t,j}(g/day)} \cdot \mathrm{CB1_{j}} \cdot \left(\frac{\mathrm{Kd_{5j}}}{\mathrm{Kd_{5j}{+}Kp_{j}}}\right) \; \forall t, j \tag{C.63}$$

$$\mathrm{RDCB2_{t,j}(g/day){=}It_{t,j}(g/day)} \cdot \mathrm{CB2_{j}} \cdot \left(\frac{\mathrm{Kd_{6j}}}{\mathrm{Kd_{6j}{+}Kp_{j}}}\right) \; \forall t, j \tag{C.64}$$

$$\mathrm{RECA_{t,j}(g/day)}=\mathrm{It_{t,j}(g/day)}\cdot \mathrm{CA_j}\cdot \left(\frac{\mathrm{Kp_j}}{\mathrm{Kd_{4j}}+\mathrm{Kp_j}}\right)\ \forall t,j \tag{C.65}$$

$$\mathrm{RECB1_{t,j}(g/day)}=\mathrm{It_{t,j}(g/day)}\cdot \mathrm{CB1_j}\cdot \left(\frac{\mathrm{Kp_j}}{\mathrm{Kd_{5j}}+\mathrm{Kp_j}}\right)\ \forall t,j \tag{C.66}$$

$$\mathrm{RECB2_{t,j}(g/day)}=\mathrm{It_{t,j}(g/day)}\cdot \mathrm{CB2_j}\cdot \left(\frac{\mathrm{Kp_j}}{\mathrm{Kd_{6j}}+\mathrm{Kp_j}}\right)\ \forall t,j \tag{C.67}$$

Calculation of Microbial Yield for carbohydrate fermenting.

The bacterial decomposition performance of the fiber, sugar, and starch fraction ($Y1_j$, $Y2_j$, $Y3_j$) is calculated using Eqs.(C.68)-(C.70), where YG_1, YG_2 are 0.4 and KM_1, KM_2 are 0.05 and 0.15, respectively.

$$\frac{1}{\mathrm{Y1_j}}=\frac{\mathrm{KM_1}}{\mathrm{Kd_{6j}}}+\frac{1}{\mathrm{YG_1}}\ \forall j \tag{C.68}$$

$$\frac{1}{\mathrm{Y2_j}}=\frac{\mathrm{KM_2}}{\mathrm{Kd_{4j}}}+\frac{1}{\mathrm{YG_2}}\ \forall j \tag{C.69}$$

$$\frac{1}{\mathrm{Y3_j}}=\frac{\mathrm{KM_2}}{\mathrm{Kd_{5j}}}+\frac{1}{\mathrm{YG_2}}\ \forall j \tag{C.70}$$

Using these yields it is possible to estimate the amount of bacteria generated ($BACT_{t,j}$) using equation Eq.(C.71).

$$\mathrm{BACT_{t,j}}=\mathrm{NFCBACT_{t,j}}+\mathrm{FCBACT_{t,j}}\ \forall t,j \tag{C.71}$$

The sources of bacteria are two, fiber and non-fiber carbohydrate bacteria ($FCBACT_{t,j}$ and $NFCBACT_{t,j}$). These are calculated using Eq.(C.72) and (C.73) respectively.

$$\mathrm{FCBACT_{t,j}(g/day)}=\mathrm{Y1_j}\cdot \mathrm{RDCB2_{t,j}(g/day)}\ \forall t,j \tag{C.72}$$

$$\mathrm{NFCBACT_{t,j}(g/day)}=(\mathrm{Y_2}\cdot \mathrm{RDCA_{t,j}(g/day)})+(\mathrm{Y_3}\cdot \mathrm{RDCB1_{t,j}(g/day)})\ \forall t,j$$

(C.73)

With regard to the nitrogen balance associated with bacteria, the different existing sources must be considered. The nitrogen present in bacteria ($BACTN_{t,j}$), in bacterial fiber carbohydrate ($FCBACTN_{t,j}$) and non-fiber carbohydrate ($NFCBACTN_{t,j}$) represents 10% of each of them (Eqs.(C.74)-(C.76)).

$$\mathrm{BACTN_{t,j}(g/day){=}0.1 \cdot BACT_{t,j}(g/day)}\ \forall t,j \tag{C.74}$$

$$\mathrm{NFCBACTN_{t,j}(g/day){=}0.1 \cdot NFCBACT_{t,j}(g/day)}\ \forall t,j \tag{C.75}$$

$$\mathrm{FCBACTN_{t,j}(g/day){=}0.1 \cdot FCBACT_{t,j}(g/day)}\ \forall t,j \tag{C.76}$$

All the degraded amount of proteins in the rumination phase ($REPEP_{t,j}$) becomes part of bacterial peptide ($PEPUP_{t,j}$) (Eq.(C.77)). Eq.(C.78) calculates of the nitrogen part of the bacterial peptide ($PEPUPN_{t,j}$).

$$\mathrm{PEPUP_{t,j}(g/day){=}RDPEP_{t,j}(g/day)}\ \forall t,j \tag{C.77}$$

$$\mathrm{PEPUPN_{t,j}(g/day){=}PEPUP_{t,j}(g/day)/6.25}\ \forall t,j \tag{C.78}$$

With the previously calculated variables and the rest that were already known, it is possible to carry out a nitrogen and peptide balance. The excess nitrogen of the bacterial rumen (EN) is given by Eq.(C.79), the bacterial nitrogen balance ($BACTNBAL_{t,j}$) is estimated by Eq.(C.80) and the peptide balance ($PEPBAL_{t,j}$) is shown in Eq.(C.81). U is the ruminant nitrogen usage and is predicted by Eq.(C.82).

$$\begin{gathered}\mathrm{EN_t(g/day){=}\sum_j PEPUPN_{t,j}(g/day){+}\frac{\sum_j RDPA_{t,j}(g/day)}{6.25}+} \\ \left(\frac{\mathrm{\sum_j MPa_{t,j}(g/day)\text{-}MPreq_t(g/day)}}{6.25}\right) - \sum_j \mathrm{BACTN_{t,j}(g/day)}\ \forall t\end{gathered} \tag{C.79}$$

$$\mathrm{BACTNBAL_{t,j}(g/day)=(((\frac{PEPUP_{t,j}(g/day)+RDPA_{t,j}(g/day))}{6.25})+ U_j(g/day))\text{-}BACTN_{t,j}(g/day)}\ \forall t,j \tag{C.80}$$

$$\mathrm{PEPBAL_{t,j}(g/day)=\frac{PEPUP_{t,j}(g/day)}{6.25}\text{-}(2/3)\cdot NFCBACTN_{t,j}(g/day)}\ \forall t,j \tag{C.81}$$

$$\mathrm{U_j=121.7\text{-}12.01\cdot CP_j+0.3235\cdot CP_j{}^2}\ \forall j \tag{C.82}$$

The bacterial composition in terms of carbohydrates ($REBCHO_{t,j}$), fat ($REBFAT_{t,j}$), true protein ($REBTP_{t,j}$), bacterial cell wall protein ($REBCW_{t,j}$), bacterial nucleic acids and ashes ($REBNA_{t,j}$) is estimated by Eqs.(C.83)-(C.88).

$$\mathrm{REBTP_{t,j}(g/day)=0.6\cdot 0.625\cdot BACT_{t,j}(g/day)}\ \forall t,j \tag{C.83}$$

$$\mathrm{REBCW_{t,j}(g/day)=0.25\cdot 0.625\cdot BACT_{t,j}(g/day)}\ \forall t,j \tag{C.84}$$

$$\mathrm{REBNA_{t,j}(g/day)=0.15\cdot 0.625\cdot BACT_{t,j}(g/day)}\ \forall t,j \tag{C.85}$$

$$\mathrm{REBCHO_{t,j}(g/day)=0.21\cdot BACT_{t,j}(g/day)}\ \forall t,j \tag{C.86}$$

$$\mathrm{REBFAT_{t,j}(g/day)=0.12\cdot BACT_{t,j}(g/day)}\ \forall t,j \tag{C.87}$$

$$\mathrm{REBASH_{t,j}(g/day)=0.044\cdot BACT_{t,j}(g/day)}\ \forall t,j \tag{C.88}$$

Intestinal digestion process.

During this phase, a percentage of the proteins, carbohydrates and fats that were not digested in the rumination phase are assimilated. The amount of digestible protein B1, B2 and B3 ($DIGPB1_{t,j}$, $DIGPB2_{t,j}$ and

$DIGPB3j_{t,j}$, respectively) in the intestinal digestion process is calculated by Eqs.(C.89)-(C.91). The total amount of digestible protein from the diet ($DIGFP_{t,j}$) is calculated by Eq.(C.92).

$$\mathrm{DIGPB1_{t,j}(g/day){=}REPB1_{t,j}(g/day)}\ \forall t, j \tag{C.89}$$

$$\mathrm{DIGPB2_{t,j}(g/day){=}REPB1_{t,j}(g/day)}\ \forall t, j \tag{C.90}$$

$$\mathrm{DIGPB3_{t,j}(g/day){=}0.8 \cdot REPB3_{t,j}(g/day)}\ \forall t, j \tag{C.91}$$

$$\begin{aligned}&\mathrm{DIGFP_{t,j}(g/day){=}DIGPB1_{t,j}(g/day){+}DIGPB2_{t,j}(g/day){+}}\\&\mathrm{DIGPB3_{t,j}(g/day)}\ \forall t, j\end{aligned} \tag{C.92}$$

The sources of bacterial protein are two, the digestible bacterial true protein ($DIGBTP_{t,j}$) and the digestible bacterial nucleic acids ($DIGBNA_{t,j}$). They are calculated by Eq.(C.93) and Eq.(C.94), respectively.

$$\mathrm{DIGBTP_{t,j}(g/day){=}REBTP_{t,j}(g/day)}\ \forall t, j \tag{C.93}$$

$$\mathrm{DIGBNA_{t,j}(g/day){=}REBNA_{t,j}(g/day)}\ \forall t, j \tag{C.94}$$

The total amount of protein is shown in Eq.(C.95).

$$\mathrm{DIGP_{t,j}{=}DIGFP_{t,j}{+}DIGBTP_{t,j}{+}DIGBNA_{t,j}}\ \forall t, j \tag{C.95}$$

The digested carbohydrates in the intestines from food ($DIGFC_{t,j}$) are calculated by Eq.(C.96), where stdig is the postruminal starch digestibility. The carbohydrates obtained from the digestion of bacteria ($DIGBC_{t,j}$) is calculated by Eq.(C.97). The total amount of digested carbohydrates ($DIGC_{t,j}$) is shown by Eq.(C.98).

$$\begin{aligned}&\mathrm{DIGFC_{t,j}(g/day){=}RECA_{t,j}(g/day){+}stdig \cdot RECB1_{t,j}(g/day)}\\&\mathrm{{+}0.2 \cdot RECB2_{t,j}(g/day)}\ \forall t, j\end{aligned} \tag{C.96}$$

$$\mathrm{DIGBC_{t,j}(g/day){=}0.95 \cdot REBCHO_{t,j}(g/day)}\ \forall t, j \tag{C.97}$$

$$\mathrm{DIGC_{t,j}(g/day)=DIGFC_{t,j}(g/day)+DIGBC_{t,j}(g/day)}\ \forall t,j \tag{C.98}$$

Lastly, it will be necessary to calculate how much fat is digested in the intestine. The fat is not digested in the rumination phase, so it passes in its entirety to the intestine ($REFAT_{t,j}$) as indicated in Eq.(C.99).

$$\mathrm{REFAT_{t,j}(g/day)=It_{t,j}(g/day)\cdot FAT_{t,j}}\ \forall t,j \tag{C.99}$$

In the same way as in the previous cases, the digested fat in the intestines has two sources, the diet ($DIGFF_{t,j}$) and the bacteria formed in the previous phase ($DIFBF_{t,j}$). The estimation of both sources is indicated in Eqs.(C.100) and (C.111), while the sum ($DIGF_{t,j}$) is calculated by Eq.(C.102).

$$\mathrm{DIGFF_{t,j}(g/day)=0.95\cdot REFAT_{t,j}(g/day)}\ \forall t,j \tag{C.100}$$

$$\mathrm{DIGBF_{t,j}(g/day)=0.95\cdot REBFAT_{t,j}(g/day)}\ \forall t,j \tag{C.101}$$

$$\mathrm{DIGF_{t,j}(g/day)=DIGFF_{t,j}(g/day)+DIGBF_{t,j}(g/day)}\ \forall t,j \tag{C.102}$$

Composition of waste.

The waste expelled by livestock is made up of all the nutrients that have not been digested in previous phases. The sum of the undigested proteins ($FEFP_{t,j}$) is composed of the undigested part of the proteins B3 ($FEPB3_{t,j}$) and C ($FEPC_{t,j}$) and are calculated in Eqs.(C.103)-(C.105).

$$\mathrm{FEFP_{t,j}(g/day)=FEPB3_{t,j}(g/day)+FEPC_{t,j}(g/day)}\ \forall t,j \tag{C.103}$$

$$\mathrm{FEPB3_{t,j}(g/day)=(1\text{-}0.8)\cdot REPB3_{t,j}(g/day)}\ \forall t,j \tag{C.104}$$

$$\mathrm{FEPC_{t,j}(g/day)=REPC_{t,j}(g/day)}\ \forall t,j \tag{C.105}$$

In the case of carbohydrates, the sum ($FEFC_{t,j}$) is made up of starch ($FECB1_{t,j}$), available fiber ($FECB2_{t,j}$), unavailable fiber ($FECC_{t,j}$) and the amounts of these are estimated by Eqs.(C.106)-(C.109).

$$\begin{aligned}&\mathrm{FEFC_{t,j}(g/day)=FECB1_{t,j}(g/day)+}\\&\mathrm{FECB2_{t,j}(g/day)+FECC_{t,j}(g/day)}\ \forall t,j\end{aligned} \tag{C.106}$$

$$\text{FECB1}_{\text{t,j}}(\text{g/day})=(\text{1-stdig}) \cdot \text{RECB1}_{\text{t,j}}(\text{g/day}) \ \forall t, j \tag{C.107}$$

$$\text{FECB2}_{\text{t,j}}(\text{g/day})=(\text{1-0.2}) \cdot \text{RECB2}_{\text{t,j}}(\text{g/day}) \ \forall t, j \tag{C.108}$$

$$\text{FECC}_{\text{t,j}}(\text{g/day})=\text{RECC}_{\text{t,j}}(\text{g/day}) \ \forall t, j \tag{C.109}$$

Fat only has one source (FEFF_j) and is estimated by Eq.(C.110), as in the case of ashes that are not digested in any other phase and therefore, expelled with the feces (FEFA_j), its quantity being calculated by Eq.(C.111).

$$\text{FEFF}_{\text{j}}(\text{g/day})=\text{REFAT}_{\text{j}}(\text{g/day}) \cdot (\text{1-0.95}) \ \forall j \tag{C.110}$$

$$\text{FEFA}_{\text{j}}(\text{g/day})=\text{It}_{\text{j}}(\text{g/day}) \cdot \text{ASH}_{\text{j}} \cdot (\text{1-0.5}) \ \forall j \tag{C.111}$$

Microbial matter in the feces

Through the bacterial composition of feces, the total amount of proteins, carbohydrates and fats that come from bacteria and are present in the feces can be determined. On the one hand, the amount of fecal bacterial cell wall protein ($\text{FEBCW}_{t,j}$) and the amount of fecal bacterial protein ($\text{FEBCP}_{t,j}$) are estimated by Eqs.(C.112)-(C.113). On the other hand, the amount of bacterial carbohydrate ($\text{FEBC}_{t,j}$), fat ($\text{FEBF}_{t,j}$) and ash ($\text{FEBASH}_{t,j}$) are calculated by Eqs.(C.114)-(C.116). The sum of all the amount of bacteria present in the feces ($\text{FEBACT}_{t,j}$) is given by Eq.(C.117).

$$\text{FEBCW}_{\text{t,j}}(\text{g/day})=\text{REBCW}_{\text{t,j}}(\text{g/day}) \ \forall t, j \tag{C.112}$$

$$\text{FEBCP}_{\text{t,j}}(\text{g/day})=\text{FEBCW}_{\text{t,j}}(\text{g/day}) \ \forall t, j \tag{C.113}$$

$$\text{FEBC}_{\text{t,j}}(\text{g/day})=(\text{1-0.95}) \cdot \text{REBCHO}_{\text{t,j}}(\text{g/day}) \ \forall t, j \tag{C.114}$$

$$\text{FEBF}_{\text{t,j}}(\text{g/day})=(\text{1-0.95}) \cdot \text{REBFAT}_{\text{t,j}}(\text{g/day}) \ \forall t, j \tag{C.115}$$

$$\mathrm{FEBASH_{t,j}(g/day)=(1\text{-}0.5)\cdot REBASH_{t,j}(g/day)}\ \forall t,j \tag{C.116}$$

$$\begin{aligned}&\mathrm{FEBACT_{t,j}(g/day)=FEBCW_{t,j}(g/day)+FEBCP_{t,j}(g/day)}\\&\mathrm{+FEBC_{t,j}(g/day)+FEBF_{t,j}(g/day)+FEBASH_{t,j}(g/day)}\ \forall t,j\end{aligned} \tag{C.117}$$

There is a certain amount of proteins ($\mathrm{FEENGP}_{t,j}$), fats ($\mathrm{FEENGF}_{t,j}$) and ashes ($\mathrm{FEENGA}_{t,j}$) that are endogenously generated. This quantity is estimated by Eqs.(C.118)-(C.120).

$$FEENG\mathrm{P_{t,j}(g/day)=0.09\cdot IDM_{t,j}(kg/day)\cdot 1000g/kg}\ \forall t,j \tag{C.118}$$

$$\mathrm{FEENGF_{t,j}(g/day)=0.0119\cdot DMI_{t,j}(g/day)\cdot 1000g/kg}\ \forall t,j \tag{C.119}$$

$$\mathrm{FEENGA_{t,j}(g/day)=0.017\cdot DMI_{t,j}(g/day)\cdot 1000g/kg}\ \forall t,j \tag{C.120}$$

Summing all protein sources ($\mathrm{FEPROT}_{t,j}$) in Eq.(C.121), carbohydrates ($\mathrm{FECHO}_{t,j}$) in Eq.(C.122), fats ($\mathrm{FEFAT}_{t,j}$) in Eq.(C.123) and ashes ($\mathrm{FEASH}_{t,j}$) in Eq.(C.124) gives the total amount of waste generated ($\mathrm{FEDM}_{t,j}$), calculated by Eq.(C.125).

$$\begin{aligned}&\mathrm{FEPROT_{t,j}(g/day)=FEFP_{t,j}(g/day)+}\\&\mathrm{FEBCP_{t,j}(g/day)+FEENGP_{t,j}(g/day)}\ \forall t,j\end{aligned} \tag{C.121}$$

$$\mathrm{FECHO_{t,j}(g/day)=FEFC_{t,j}(g/day)+FEBC_{t,j}(g/day)}\ \forall t,j \tag{C.122}$$

$$\begin{aligned}&\mathrm{FEFAT_{t,j}(g/day)=FEBF_{t,j}(g/day)+FEFF_{t,j}(g/day)+}\\&\mathrm{FEENGF_{t,j}(g/day)}\ \forall t,j\end{aligned} \tag{C.123}$$

$$\begin{aligned}&\mathrm{FEASH_{t,j}(g/day)=FEFA_{t,j}(g/day)+}\\&\mathrm{FEBASH_{t,j}(g/day)+FEENGA_{t,j}(g/day)}\ \forall t,j\end{aligned} \tag{C.124}$$

$$\mathrm{FEDM_{t,j}(g/day)=}\left(\frac{\mathrm{FEFP_{t,j}(g/day)+FEBCP_{t,j}(g/day)+FECHO_{t,j}(g/day)+FEFAT_{t,j}(g/day)+FEASH_{t,j}(g/day)}}{0.91}\right)\forall t,j \tag{C.125}$$

All the equations of the model are adapted to be integrated into GAMS.

C.2 waste treatment and nutrient recovered systems

The composition of the manure is used to determine the amount of biogas and digestate that can be produced. This depends on the feed and a kinetic model based on the studies from the literature (Taifouris et al., 2021). The empirical formulas for lipids, proteins, and carbohydrates are used to compute the energy and mass balances using the following reactions:

Lipids:

$C_{57}H_{104}O_6$+23.64 H_2O+1.45NH_3 $\rightarrow$ 36.36CH_4+13.34 CO_2+1.45 $C_5H_7NO_2$

Protein:

$CH_{2.03}$ $O_{0.6}N_{0.3}S_{0.001}$+0.31 H_2O $\rightarrow$ 0.41 CH_4+0.42 CO_2+0.030$C_5H_7NO_2$ +0.001H_2S+0.26NH_3

Carbohydrates:

$C_6H_{10}O_5$+0.35 H_2O+0.22 NH_3 $\rightarrow$ 2.46 CH_4+2.46CO_2+0.22$C_5H_7NO_2$

It is considered that the kinetics follows a first-order reaction, where hydrolysis is the limiting phase and that a stirred isothermal batch reactor is used to carry out the reaction (Taifouris & Martín, 2018). The residence time and the conversion under those conditions are 24 days and 0.51, respectively (Kafle & Chen, 2016). The Dalton's and Raoult's principles, as well as Antoine's equation, are used to determine the gas and liquid composition exiting the reactor.

Different technologies for the purification of biogas can be combined to obtain energy through its combustion, such as a bed of Fe_2O_3 to remove the H_2S, a scrubber to reduce ammonia content down to 5%, and a pressure swing adsorption system to remove the water, 95% of the CO_2 and the rest of the ammonia (León & Martín, 2016). The liquid and solid effluents are separated using a decanter centrifuge. The solid retained 25% of ammonia and this is lost in the storage. The NH3 is recovered by ammonia stripping process with a yield of 0.89, consuming 27.7gCa $(OH)_2$ per liter of effluent and 2.88 kg of H2SO4 per kilogram of NH_3. The rest of nutrient are totally recovered. The mass balance of the recovered nutrient is estimated by Eqs.C.126-(C.128).

$$N_{rec}= \sum_t 0.89 \cdot NH_{3_{1t}} \tag{C.126}$$

$$P_{rec}=\sum_t Psup_{feed_t}+ Psup_{supp_t}- P_{nd_t} \tag{C.127}$$

$$K_{rec}=\sum_t \; Ksup_{feed_t}- K_{nd_t} \tag{C.128}$$

NH_3l is the ammonia present in the non-gaseous phase of the effluent that leaves the anaerobic digestion reactor. K_{nd} and P_{nd} are the minerals necessary for the growth and maintenance of the animals, while $Ksup_{feedt}$ and $Psup_{feedt}$ are the minerals supplied with feed and $Psup_{supp}$ is the phosphorus supplied by the supplement. The flowsheet can be seen in the Figure C.1.

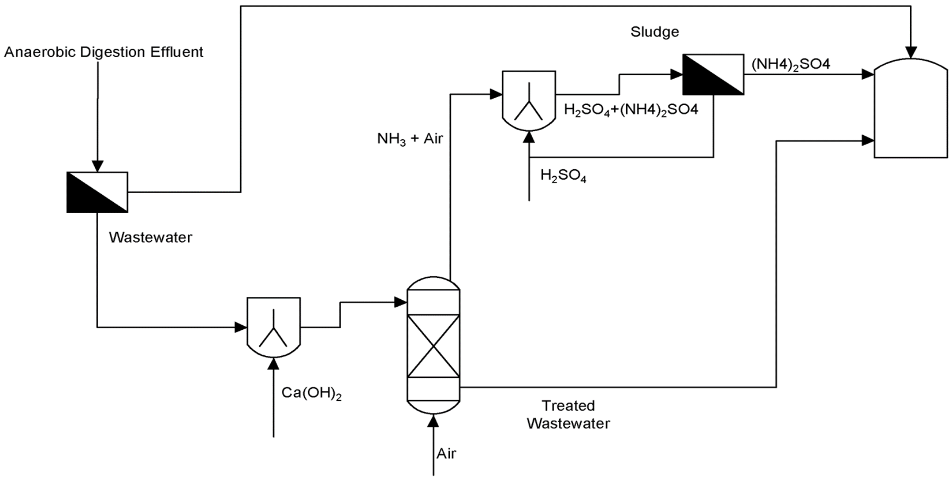

Figure C.1: Ammonia stripping process

C.3 FERTILIZER FORMULATION

The formulation of the necessary mineral fertilizer is estimated by Eqs.C.129- C.131.

$$N_{mine} \cdot x_N = N_{nd} - N_{rec} \tag{C.129}$$

$$P_{mine} \cdot x_P = P_{nd} - P_{rec} \tag{C.130}$$

$$K_{mine} \cdot x_K = K_{nd} - K_{rec} \tag{C.131}$$

Where x_N, x_P, and x_K (0.34, 0.2, and 0.5) (Agrifeed, 2021) are the composition of nitrogen, phosphorus, and potassium in the mineral fertilizer, respectively. N_{mine} is the amount of ammonium nitrate used to supply the amount of nitrogen to the system while P_{mine} is the amount of simple perphosphate. K_{mine} is the amount of potassium sulfate.

C.4 ENVIRONMENTAL IMPACT INDEX.

The global warming potential (GWP), eutrophication potential (EUp) and water footprint (WF) are shown in the Table C.1.

Table C.1: Environmental indexes of mineral nutrients (Nemecek & Erzinger, 2007; Daccache et al., 2014; Skowrońska & Filipek, 2014; Serenella et al., 2018)

	Ammonium Nitrate	**Single superphosphate**	**Potassium sulphate**	**Water used**	**Weight**
GWP ($t_{CO2-Eq}/t_{fertilizer}$)	0.93	0.12	1.02	$2.187\cdot10^{-5}$	0.65
EUp($kg_{PO4-3eq}/t_{fertilizer}$)	0.17	0.11	0.18	-	0.09
Water footprint(t)	-	-	-	1	0.26

The upper limit and the lower limits of the three different indexes are calculated to compute the composite index and are shown in the Table C.2.

Table C.2: Maximum and minimum values of the environmental indexes considered.

	Min	Max
GWP ($t_{CO2-Eq}/t_{fertilizer}$)	584	1765
Eutrophication potential($kg_{PO4-3eq}/t_{fertilizer}$)	105	395
Water footprint(m^3)	0	1314100
CI	0.17	0.74

C.5 CROPS PROPERTIES

12 different ingredients and 2 supplements are considered. On the one hand, their production yields, crop production cost (tillage, sowing and harvesting), fertilizer requirements and period can be seen in the Table C.3. On the other hand, their nutritional characteristic of the crops can be consulted in the Table C.4.

Table C.3: Production cost and fertilizer consumption of the considered crops (Bellido, 2005, 2010; El confidencial Químico, 2016; Ministerio de Agricultura pesca y alimentación, 2019; y Alimentación Ministerio de Agricultura, 2019; de León, 2020; Ministerio de agricultura pesca y alimentación, 2020; Echemi, 2021)

Crop	Period	Crop production cost(€/kg)	Production yield (kg/ha· year)	Necessary nutrients (kg/ha)	Price (€/kg)
Alfalfa	Annual	0.029112	10000	30N/240P/300K	0.168
Vetch, Hay	Winter	0.058224	5000	100N/85P/130K	0.111
Barley, Stover	Winter	0.058224	5000	100N/85P/130K	0.090
Barley, Straw	Winter	0.0612122	3272	50N/22P/100K	0.030
Wheat, Straw	Winter	0.0411382	3610	102N/41P/95K	0.030
Corn Stover	Spring	0.019408	15000	190N/120P/220K	0.090
Oat hay	Winter	0.0864996	1617	44N/19P/39K	0.173
Corn Grain	Spring	0.0231775	12000	259N/120P/240K	0.233
Sorgo	Spring	0.058224	5000	95N/85P/110K	0.171
Barley Grain	Winter	0.0612122	3272	50N/22P/100K	0.190
Wheat Grain	Winter	0.0411382	3610	102N/41P/95K	0.215
Rye grain	Winter	0.0796980	1755	33N/22P/32K	0.172
Calcium Carbonate	-	-	-	-	0.065
Mono-Sodium Phosphate	-	-	-	-	1.2

Table C.4: Nutritional and energy characteristic of the considered ingredients (Council, 2000)

Crop	Alfalfa	Vecth	Barley Stover	Barley Straw	Corn stover	Wheat Straw	Oat hay	Corn Grain	Barley GRain	Wheat Grain	Rye GRain	Sorghum
Type	Forage							Concentrate				
DM(%AF)	38.0	89	91	91	25	89	92.2	88	92	90	88	70
NDF(%DM)	47.00	48	72.5	72.5	60	78.9	74.4	9	28	9.7	19	23
Lignin(%NDF)	23.40	16.67	13.75	13.75	5	16.47	20	2.22	20.8	4.29	5.3	6.09
eNDF(%NDF)	82	92	100	100	81	98	98	0	36	2.6	34	34
TDN(%DM)	58.0	57	40	40	65	41.0	45	88	75	85	84	88
ME(Mcal/kg)	2.10	2.06	1.45	1.45	2.35	1.48	1.63	3.18	2.71	3.07	3.04	2.75
NEm(Mcal/kg)	1.24	1.21	0.6	0.60	1.47	0.64	0.79	2.18	1.79	2.09	2.06	1.82
Neg(Mcal/kg)	0.68	0.64	0.08	0.08	0.88	0.11	0.25	1.5	1.16	1.42	1.4	1.19
CP(%DM)	17	20.8	4.4	4.4	9	3.5	4.4	9.8	48.9	11.3	13.8	12.40
DIP(%CP)	91.0	86	30	30	78	31	55	57.4	57	74	79	50.8
solCP(%CP)	45.0	28	20	20	45	20	20	11	20	30	53	12.0
NPN(%SolCP)	100.00	96	95	95	100	95	95	73	40	73	19	33
NDFIP(%CP)	32.00	25.2	75	75	16	75	75	15	10	4	7	10
ADPIP(%CP)	18.00	14	65	65	4.5	65	65	5	8	2	4	5
Starch(%NSC)	89	60	100	100	80	100	5	90	90	90	90	90
Fat(%DM)	3.10	3	1.9	1.9	3.1	2	2.2	4.3	1.7	1.9	1.7	3.10
Ash(%DM)	9.00	7	7.5	7.5	11	7.7	7.8	1.6	7	2	2	2
KCA (hr-1)	10	250	250	250	10	250	250	250	300	300	300	150
KC1(hr-1)	25	30	30	30	30	50	30	25	25	40	40	10
KC2(hr-1)	5.5	5.S	3	3.0	4	3	3	6	6	6	8	5.0
KB1(hr-1)	150	150	135	135	300	135	135	135	175	300	300	135
KB2(hr-1)	11	9	11	11	10	11	11	10	8	12	12	6
KB3(hr-1)	1.75	1.25	0.09	0.09	0.2	0.09	0.09	0.1	0.25	0.35	0.35	0.12
Ca(%DM)	1.74	1.36	0.3	0.3	0.52	0.17	0.23	0.03	0.16	0.07	0.07	0.05
P(%DM)	0.27	0.34	0.07	0.07	0.31	0.05	0.06	0.31	0.76	0.33	0.36	0.34
Mg(%DM)	0.33	0.27	0.23	0.23	0.31	0.12	0.17	0.11	0.35	0	0.14	0.14
CI(%DM)	0.41	0	0.67	0.67	0	0.32	0.78	0.06	0	11	0.03	0.09
K(%DM)	2.35	2.12	2.37	2.37	1.64	1.41	2.53	0.33	1.22	0	0.52	0.47
Na(%DM)	0.16	0.52	0.14	0.14	0	0.14	0.42	0.01	0.03	0.43	0.03	0.04
S(%DM)	0.31	0.15	0.17	0.17	0	0.19	0.22	0.14	0.26	0.02	0.17	0.12

C.6 SOLUTION PROCEDURE

The income from the sale of meat of cows (In_{cows}), male yearling ($In_{YearlingM}$) and female yearling ($In_{YearlingF}$) are estimated by Eqs.(C.132)-(C.134).

$$In_{Cows}= (NA_{Cows}) \cdot Pri_{Cow} \tag{C.132}$$

$$In_{YearlingM}= (NA_{YearlingM}) \cdot Pri_{YearlingM} \tag{C.133}$$

$$In_{YearlingF}= (NA_{YearlingF}) \cdot Pri_{YearlingF} \tag{C.134}$$

The price of yearlings ($Pri_{YearlingM}$ and $Pri_{YearlingF}$) can be estimated using its final weight, meat yield (Huerta-Leidenz et al., 2013), and the official price of the meat from the literature, whereas the price of the cows (Pri_{Cow}) is fixed, 504€/cow. $Pri_{yearlingM}$ is 516€/yearling and $Pri_{yearlingF}$ is 685€/yearling (Lonja de Salamanca, 2021). NA_{cows}, $NA_{YearlingM}$, and $NA_{YearlingF}$ are the number of cows, male yearling and female yearling, respectively. Pot is calculated by Eq.(C.135), where Cst_{Calves} is growing cost of calves and $Cst_{Yearling}$ is the growing cost of the yearling. Pri_{Animal} is the price of the animal, whose value can be $Pri_{YearlingM}$ for male calves or $Pri_{YearlingF}$ for female calves.

$$Pot= Pri_{Animal}- Cst_{Calves}- Cst_{Yearling} \tag{C.135}$$

The growing cost of calves, yearlings, cows, and bulls are calculated by Eqs.(C.136)-(C.139).

$$Cst_{Calves}= \sum_{t=0}^{6} DMI_t \cdot CstM_t \cdot NA_{calves} \tag{C.136}$$

$$Cst_{Yearling}= \sum_{t=7}^{20} DMI_t \cdot CstM_t \cdot NA_{yearling} \tag{C.137}$$

$$Cst_{Cow}= \sum_{t=21}^{72} DMI_t \cdot CstM_t \cdot NA_{cows} \tag{C.138}$$

$$\mathrm{Cst_{Bulls}} = \sum_{t=21}^{72} \mathrm{DMI_t} \cdot \mathrm{CstM_t} \cdot \mathrm{NA_{Bulls}} \tag{C.139}$$

Where $CstM_t$ is the crop production cost of feed in the period 't' and DMI_t (Kg/TU) is the amount of dry matter intake in a time period 't'. NA_{calves}, $NA_{yearling}$, NA_{bulls} are the number of calves, yearlings, and bulls, respectively. $CstM_t$ is calculated by Eq.(C.140) .

$$\mathrm{CstM_t} = \sum_{j} \mathrm{x_{t,j}} \cdot \mathrm{Cst_j} \ \forall t \tag{C.140}$$

Where Cst_j corresponds to the crop production cost of the ingredient "j" and can be consulted in Table C.3. This cost is the acquisition costs (the parameter "price" of the Table S.3) in the case of the non-integrated livestock. $x_{t,j}$ is the part of the ingredient 'j' in the period 't' in the feed.

The auxiliary costs are calculated by Eqs.(C.141)-(C.145).

$$\mathrm{Cst_{waterAgri}} = \mathrm{Cst_{WaterCorn}} \cdot \mathrm{A_{corn}} \tag{C.141}$$

Where $Cost_{WaterCorn}$ is 1100€ per hectare of corn and A_{corn} is the area of corn (de Valladolid, 2018).

$$\begin{aligned} \mathrm{Cst_{waterLiv}} = {} & \mathrm{Wa_{Calves}} \cdot \mathrm{NA_{Calves}} \cdot \mathrm{lt_{Calves}} + \mathrm{Wa_{Yearling}} \cdot \mathrm{NA_{Yearling}} \cdot \mathrm{lt_{Yearling}} + \\ & \mathrm{Wa_{cows}} \cdot \mathrm{NA_{cows}} \cdot \mathrm{lt_{cows}} \end{aligned} \tag{C.142}$$

Where Wa_{Calves}, $Wa_{yearling}$, and Wa_{Cows} are the consumption of water per day of calves, yearling and cows and their values are 3.5, 25, 70 l/day, (Lanuza A, 2006; Duarte, 2011) respectively. lt_{calves}, $lt_{Yearling}$ and It_{cows} are the lifetime of those animals that can be consulted in Figure 5.1.

$$\mathrm{Cst_{Supl}} = \mathrm{Amt_{supP}} \cdot \mathrm{Price_{supP}} + \mathrm{Amt_{supCa}} \cdot \mathrm{Price_{supCa}} \tag{C.143}$$

Where the price of mono-sodium phosphate (Pri_{supP}) is € 1.2 / kg (Echemi, 2021) and the price of calcium carbonate (Pri_{supCa}) is € 0.065 / kg (El confidencial Químico, 2016).

$$\mathrm{Cst_{Bass}} = \mathrm{Amt_{Ca(OH)_2}} \cdot \mathrm{Pri_{Ca(OH)_2}} \tag{C.144}$$

$$Cst_{Acid} = Amt_{H_2SO_4} \cdot Pri_{H_2SO_4} \tag{C.145}$$

Where the cost of calcium hydroxide ($Pri_{Ca(OH)2}$) and acid ($Pri_{H_2SO_4}$) are € 256 / t (Alibaba, 2021), € 70 / t, respectively.

C.7 TRANSPORTATION COST OF THE NON-INTEGRATED CASE.

The transportation cost is calculated for the non-integrated case. The calculation of transport costs was carried out taking into account the following considerations:

- A distance of 20 km is considered for the calculation.
- It is considered that the forages will be packed in rectangular blocks that have a density of 200kg / m3 (Organización de las naciones unidas para la agricultura y la alimentación, 2003)
- 2 and 5 axle trucks may be used depending on the total quantity to be transported.
- 2-axle trucks have a useful volume of $75m^3$, while 5-axle trucks have a volume of 111^3. The maximum load also depends on the number of axles, being 18 tm in the case of 2-axle trucks and 25 tm. tm in those of 5 (Movilidad y Agenda Urbana Ministerio de Transportes, 2021)
- Depending on the type of truck, the cost per kilometer traveled, with a full truck and an empty truck, can be consulted in the bibliography (Movilidad y agenda urbana Ministerio de transporte, 2021)

First it will be necessary to determine the number of trips that must be made by the trucks. The average distance of the trips is considered to be 20 km. The limit of the truck can be given by the maximum available volume (especially in forages) or the maximum load. The total number of kilometers traveled by full and empty trucks is established and multiplied by the transport costs consulted in the bibliography. The number of full and empty trucks is the same the results of the calculations can be consulted in Table C.5.

Table C.5: Economic evaluation of tansport cost

Crop	Ton	Number of Trucks	Km	Full trucks cost (€)	Empty trucks cost (€)	Total transport cost (€)
Alfafa	69	6.0	240	140	111	252
Vetch	122	12.0	480	280	223	504
Rye	72	6.0	240	140	111	252
Barley Grain	730	30.0	1200	756	642	1398
Sorgo	411	18.0	720	453	385	839
Barley Straw	4524	186.0	7440	4687	3980	8668
Wheat Straw	1935	78.0	3120	1965	1669	3635
Wheat Grain	1968	84.0	3360	2116	1797	3914

C.8 TECHNO-ECONOMIC EVALUATION OF THE CONSIDERED SCENARIOS

A techno-economic evaluation of the economic, multi-objective and ecofriendly scenarios is carried out and shown in Table C.6.

Table C.6: Techno-economic evaluation of the different considered scenarios

Variable	Ecofriendly Case	Multi-objective Case	Economic Case	Non-Integrated Livestock
Income (M€)				
Meat Income	0.590	0.590	0.590	0.590
Potential Income	0.810	0.810	0.810	0.810
Crops Income	1.320	1.550	1.690	0.000
Biogas Income	0.070	0.060	0.060	0.000
Total	2.790	3.010	3.150	1.390
Cost(M€)				
CostField	0.145	0.1750	0.180	0.000
Fertilizer cost	0.353	0.470	0.600	0.000
CostStorage	0.041	0.041	0.041	0.000
CostManpower	0.107	0.123	0.131	0.000
CostCrops	1.000	1.180	1.160	0.240
Suplement Cost	0.090	0.053	0.046	0.050
Aux Cost	0.255	0.070	0.060	0.040
Transport Cost	0.000	0.000	0.000	0.020
Cost of raising bulls	0.020	0.020	0.020	0.010
Total	2.010	2.130	2.240	0.360
Profit(M€)				
Total	0.780	0.880	0.910	1.030
Amount(t)				
Amount Alfalfa	2212	6	579	69.11
Amount Vetch	42	44	64	122
Amount Barley Straw	4693	5248	5476	4520
Amount Barley Grain	401	378	0	730
Amount Barley 2	1442	2816	742	0
Amount Sorgo	0	0	0	412
Amount Corn 1	0	124	1398	0
Amount Corn 4	1077	0	0	0
Amount Wheat(Grain)	0	1121	1476	1968
Amount Wheat(Straw)	0	0	0	1940
Amount Rye	0		124	72
Fertilizer (t)				
N	287	592	695	864
P	716	688	879	885
K	320	371	534	839
Total	1323	1651	2108	2588
Indexes				
GWP(tCO2)	678	1011	1297	1765
EUp(kgPO4-3eq)	185	243	311	395
Meat(t) (consumer benefit)	443(128.47)			
GWP(tCO2/tmeat)	5.270	7.870	10.100	13.730
Composite Index	0.180	0.280	0.460	0.740

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D

APPENDIX D: SUPPLEMENTARY INFORMATION OF CHAPTER 6

D.1 ESTIMATION OF LIVESTOCK NUTRITIONAL AND ENERGY REQUIREMENTS

This model is similar to the reference study (Taifouris & Martin, 2021) yet introducing the different population groups of animals growing simultaneously.

D.1.1 *Preliminary calculations of the optimization model*

By restructuring the previous model (Taifouris & Martin, 2021) it is possible to estimate a large number of variables outside the optimization model and introduce them as parameters. These variables depend on the weight of the animal (BW_t) or some variable that is dependent on it. If it is known how the weight of the animal varies with life cycle of the animals, these variables can be estimated without using the optimization framework. The variation of animal weight is known since the ideal pregnancy weight (TPW) and calving weight (TCW), as well as the ideal pregnancy age (TPA) are known. Besides, the shruck body weight (SBW_t) is estimated from the BW_t (Eq.(D.1)).

$$\mathrm{SBW_t}{=}0.96 \cdot \mathrm{BW_t}\ \forall t \tag{D.1}$$

Therefore, the weight that the animal should gain per unit of time (TU) before the first pregnancy ($BPADG_t$), during pregnancy ($APADG_t$) and after ($ACADG_t$) can be estimated, using Eqs.(D.2)-(D.4). Each TU corresponds to 24 days.

$$\mathrm{BPADG_t(kg/day)}{=}\frac{\mathrm{TPW(kg)\text{-}SBW_t(kg)}}{\mathrm{TPA(day)\text{-}TAGE_t(day)}}\ \forall t' \in [t' < TPA] \tag{D.2}$$

$$\mathrm{APADG_t(kg/day)}{=}\frac{\mathrm{TCW_1(kg)\text{-}TPW(kg)}}{\mathrm{280days}}\ \forall t' \in [TPA < t' < TPA + 280] \tag{D.3}$$

$$\mathrm{ACADG_t(kg/day)}{=}\frac{\mathrm{TCW_{xx}(kg)\text{-}TCW_x(kg)}}{\mathrm{CI(day)}}\ \forall t' \in [t' > TPA + 280] \tag{D.4}$$

Where TPW is 55% of mature weight (MW) and TPA is 440 days. t′ is the days. TCW1 is 80% of MW. CI is calving interval (350 days). Consequently, it is now possible to determine the weight of the animal in each TU, according to its life cycle, before Eq.(D.5), during Eq.(D.6), or after Eq.(D.7) the first pregnancy. It must be considered that each cow can have up to 3 pregnancies, so that the target weights after each pregnancy correspond to 92% (TCW2) and 96%(TCW3) of the MW.

$$BW_t = BW_{t-1} + 24 \cdot BPADG_t (kg/day)\ \forall t \tag{D.5}$$

$$BW_t = BW_{t-1} + 24 \cdot APADG_t (kg/day)\ \forall t \tag{D.6}$$

$$BW_t = BW_{t-1} + 24 \cdot ACDG_t (kg/day)\ \forall t \tag{D.7}$$

With this information, it is possible to determine the BW_t throughout the life cycle of the animals. This allows the estimation of other derived variables such as equivalent shrunk body weight (EQSBWt), the equivalent empty body weight ($EQEBW_t$), the daily gain assuming the body is empty (EBG_t) as well as the energy required to achieve these weight increases (RE_t) ,using Eqs.(D.8)-(D.11).

$$EQSBW_t(kg) = SBW_t(kg) \cdot \left(\frac{SRW(kg)}{FSBW(kg)}\right)\ \forall t \tag{D.8}$$

$$EQEBW_t(kg) = 0.891 \cdot EQSBW_t(kg) - \frac{ADGpreg_t(g)}{1000}\ \forall t \tag{D.9}$$

$$EBG_t(kg) = 0.956 \cdot SWG_t(kg) \tag{D.10}$$

$$RE_t(Mcal/day) = 0.0635 \cdot EQEBW_t(kg) \cdot 0.75 \cdot EBG_t(kg) \cdot 1.097\ \forall t \tag{D.11}$$

Where SRW (462 kg) and FSBW (557 kg) (Council, 2000a) are a reference weight and the final shrunk body weight, respectively, based on the expected final body fat.

Besides, the weight gained due to pregnancy ($ADGpreg_t$), which depends on the time of pregnancy, can be estimated with Eq.(D.12). The time of pregnancy (tpregt) can be related to the age of the cow since the time of beginning of pregnancy is fixed by TPA and the days between two pregnancies (CI).

$$\mathrm{ADGpreg_t(g)}=\mathrm{CBW(kg)}\cdot(18.28\cdot(0.02\text{-}0.0000286\cdot \mathrm{tpreg_t(day)})\cdot e^{(0.02\cdot \mathrm{tpreg_t(day)}-0.0000143\cdot \mathrm{tpreg_t(day)}^2)})\ \forall t \tag{D.12}$$

The requirement of proteins for growth (NPg_t) and for basal vital functions ($\mathrm{MPmaint}_t$) are calculated by Eqs.(D.13) and (D.14). Eq.(D.15) and (D.16) are used to calculate the metabolizable protein (MPg_t) according to the age of the animal.

$$\mathrm{NPg_t(g/day)}=\mathrm{SWG_t(kg)}\cdot(296\text{-}(29.4(\mathrm{RE_t(Mcal/day)}/\mathrm{SWG_t(kg)})))\ \forall t \tag{D.13}$$

$$\mathrm{MPmaint}_t(\mathrm{g/day}) = 3.8\cdot \mathrm{SBWt(kg)}^{0.75} \tag{D.14}$$

$$\mathrm{MPg_t(g/day)}=\frac{\mathrm{NPg_t(g/day)}}{0.834\text{-}(\mathrm{EQSBW_t(kg)}\cdot 0.00114)}\forall t\in\{t<57TU\} \tag{D.15}$$

$$\mathrm{MPg_t(g/day)}=\frac{\mathrm{NPg_t(g/day)}}{0.492}\forall t\in\{t>57TU\} \tag{D.16}$$

It is possible to estimate the EBG_t using RE_t and EQEBW_t (Eq.D.17).

$$\mathrm{EBG_t(kg)}=12.341\cdot \mathrm{EQEBW_t(kg)}^{-0.6837}\cdot \mathrm{RE_t(Mcal/day)}^{0.9116}\ \forall t \tag{D.17}$$

The energy required to meet the basal metabolic rate of animals (NEm_t) can be calculated, using Eq.(D.18), with the SBW_t and other parameters, such as the breed (BE), the lactation periods (L) and the nutrition plan (COMP). The value of L is 1.2 during lactation periods and 1 outside those periods. COMP depend on condition score (CS), whose value is fix in 5, and can be calculated by Eq.(D.19).

$$\mathrm{NEm_t(Mcal/day)}=\mathrm{SBW_t(kg)}^{0.75}\cdot((0.077(\mathrm{Mcal/day}\cdot \mathrm{kg}^{0.75})\cdot \mathrm{BE}\cdot \mathrm{L}\cdot \mathrm{COMP}) +0.0007(\mathrm{Mcal/(day}\cdot \mathrm{kg}^{0.75}\ {}^{\circ}\mathrm{C}))\cdot(20\text{-}\mathrm{T_P}))\ \forall t \tag{D.18}$$

$$\mathrm{COMP}=0.8+((\mathrm{CS}\text{-}1)\cdot 0.05) \tag{D.19}$$

Tp is the temperature of the animals (an average temperature of the region is used). The lactation periods, knowing the life cycle of the animals, are also fixed. Be is fixed in 1, since the breed of the cows to be used is not to be fixed. Extra energy is necessary for the growth of the animal inside the cow when it is pregnant (NEmpregt). This is calculated using Eq.(D.20) using the final calf weight (CBW) and an energy efficiency parameter (km). The value of CBW is 31 kg and km is 0.576.

$$\mathrm{NEmpreg_t(Mcal/day)}=\mathrm{CBW(kg)}\cdot\left(\frac{\mathrm{k_m}}{0.13}\right)\cdot \\ (0.05855\text{-}0.0000996\cdot \mathrm{tpreg_t(day)})\cdot \mathrm{e}^{(0.03233\text{-}0.0000275\cdot \mathrm{tpreg_t(day)})\cdot \mathrm{tpreg_r(day)})} \\ \forall t \tag{D.20}$$

The main change in the model of the present work with respect to that formulated in previous work consists in the calculation of dry mater intake (DMI) per time unit. In previous work, this variable is calculated using the feed energy of maintenance (NEMA), so it is a variable of that optimization model. But it is also possible to determine the DMI_t by considering the maintenance energy of each ingredient (NEMAC_j). In this way, the daily amount fed to the animal of ingredient 'j' in time unit 't' ($\mathrm{DMIf}_{t,j}$) can be determined outside the optimization framework, since SBW and NEMAC_j(Table D.6)) are known, using Eqs.(D.21)-(D.24). This is the amount that the animal would eat in period 't' if it fed on ingredient 'j'.The DMI_t, corresponding to the feed is calculated as a linear combination of the different ingredients used in the formulation.

$$\mathrm{DMIF}_{t,j}\mathrm{(kg/day)}=\left(\frac{\mathrm{SBW_t(kg)^{0.75}\cdot(0.2435\cdot NEmac_t(Mcal/day)\text{-}0.0466\cdot NEmac_t(Mcal/day)^2\text{-}0.1128))}}{\mathrm{NEmac_t(Mcal/day)}}\right)\cdot \\ \mathrm{BFAF\cdot BI\cdot ADTV\cdot TEMP1\cdot MUDI}\ \forall j,t\in\{t<7\ \ TU\} \tag{D.21}$$

$$\mathrm{DMIf}_{t,j}\mathrm{(kg/day)}=\left(\frac{\mathrm{SBW_t(kg)^{0.75}\cdot(0.2435\cdot NEmac_t(Mcal/day)\text{-}0.0466\cdot NEmac_t(Mcal/day)^2\text{-}0.0869))}}{\mathrm{NEmac_t(Mcal/day)}}\right)\cdot \\ \mathrm{BFAF\cdot BI\cdot ADTV\cdot TEMP1\cdot MUDI}\ \forall j,t\in\{t>7\ \ TU\ and\ t<22\ \ TU\} \tag{D.22}$$

$$\mathrm{DMIf}_{t,j}\mathrm{(kg/day)}=\left(\frac{\mathrm{SBW_t(kg)^{0.75}\cdot(0.04997\cdot NEmac_t{}^2(Mcal/day)+0.03840)}}{\mathrm{NEmac_t(Mcal/day)}}\right)\cdot \mathrm{TEMP1}\cdot \\ (\mathrm{MUDI}+0.2\cdot \mathrm{Yn})\ \forall j,t\in\{t>22TU\ and\, t<36TU\}\cup \\ \{t>40\ \ TU-t<54\ \ TU\}\cup\{t>58\ \ TU-t<72\ \ TU\}$$

(D.23)

$$\text{DMIf}_{t,j}(\text{kg/day})=\left(\frac{\text{SBW}_t(\text{kg})^{0.75}\cdot(0.04997\cdot\text{NEmac}_t{}^2(\text{Mcal/day})+0.04631)}{\text{NEmac}_t(\text{Mcal/day})}\right)\cdot\text{TEMP1}\cdot(\text{MUDI}+0.2\cdot\text{Yn})\ \forall j,t\in\{t>36\ \ TU\ and\ t<40\ \ TU\}\cup\{t>54\ \ TU-t<58\ \ TU\} \tag{D.24}$$

If there is any anabolic stimulant in the feed, the value of the parameter ADTV is 1, and 0.94 otherwise. TEMP1, MUD1, BFAF, BI are parameter related to temperature, hair size, body fat and breed, respectively. The temperature range of the facilities is between 5 and 15 Celsius degrees (TEMP1=1.03), the hair size is less than 10 cm (Mud1=1), a medium body fat (BFAF=0.90) and Holstein is used as breed (Bi=1). The daily milk production factor (Ynt) is to be added to these equations and is calculated with Eq.(D.25).

$$\text{Yn}_t(\text{kg/day})=\frac{\text{n}}{\text{a}\cdot\text{e}^{\text{kn}}}\ \forall t \tag{D.25}$$

n is the lactation week (which is a known parameter related to the life cycle of the animal), a is a parameter that controls how milk production rate changes with lactation, as a function of the maximum lactation quantity (PKYD) and is calculated by Eq. (D.26). Finally, k is the inverse of the lactation period (Eq.(D.27)).

$$\text{a}=\frac{1}{\text{PKYD}(\text{kg/day})\cdot\text{k e}} \tag{D.26}$$

$$\text{k}=\frac{1}{\text{T}} \tag{D.27}$$

The decrease in milk production (Ypn_t), due to pregnancy is evaluated by Eq.(D.28)

$$\text{Ypn}_t(\text{g/day})=((\text{CBW}(\text{kg})\cdot(0.001669)\cdot(0.000000211\cdot\text{tpreg}_t(\text{day}))\cdot\text{e}^{(0.0279\text{-}0.0000176\cdot\text{tpreg}_t(\text{day}))\cdot\text{tpreg}_t(\text{day}))}))\cdot 6.25\ \forall t \tag{D.28}$$

The extra amount of protein because of pregnancy (MPpreg_t) is computed by Eq.(D.29).

$$\text{MPpreg}_t(\text{g/day})=\frac{\text{Ypn}_t(\text{g/day})}{0.65}\ \forall t \tag{D.29}$$

Performing these calculations outside the original model does not only allow to reduce the number of equations and the number of variables, but also allows to avoid the implementation of nonlinear expressions, transforming the nonlinear model to a linear one.

D.1.2 *Introduction of the population groups in the optimization model.*

The variables calculated in the previous section are calculated for a life cycle of 72 TU (each animal). However, the life cycle of the farm is 240 TU . In addition, each population group of animals starts at a different point in the life cycle (see the Gantt chart in Figure D.1).

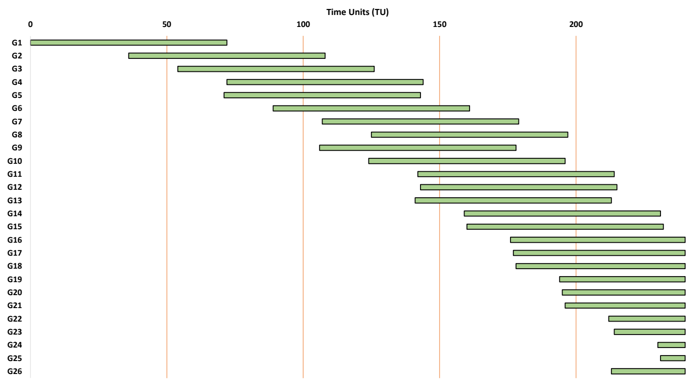

Figure D.1: .-Gantt chart of the 26 animal population groups

To integrate all population groups under the same optimization model, a vector must be defined, 'Destemporal$_{group}$'. This parameter indicates the temporal unit in which a population group is born and is shown in Table D.1. 'Destemporal$_{group}$' allows to calculate each of the variables of the model for the different population groups by establishing a conditional restriction so that the variables are only calculated in the time ranges corresponding of the corresponding group and is 0 for the rest of the time units. For example, the DMI of group 6 will only be calculated from TU 89 to TU 161, being equal to 0 for TU lower than 89 and higher than 161. This allows defining correlations only in 72-time units, while the farm cycle can have up to 240-time units.

D.1.3 *Total maintenance energy and protein requirement*

It is possible to estimate the amount of feed to supply the maintenance energy ($Im_{t,group}$) required by cattle. For this propose, the maintenance energy (NEm_t), the energy of the maintenance diet ($Nema_{t,group}$) are used in Eq.(D.30), that is added to the optimization model. If the feed contains ionophores, the value of ADTV is 1.12, otherwise its value is 1.

$$\mathrm{Im_{t,group}(kg/day)}=\frac{\mathrm{NEm_t(Mcal/day)}}{\mathrm{NEma_{t,group}(Mcal/kg)\cdot ADTV}} \ \forall t, group \qquad \text{(D.30)}$$

Table D.1: .- Life cycle of each population group

Group	Initial TU	Group	Initial TU
1	0	14	159
2	36	15	160
3	54	16	176
4	72	17	177
5	71	18	178
6	89	19	194
7	107	20	195
8	125	21	196
9	106	22	212
10	124	23	214
11	142	24	230
12	143	25	231
13	141	26	213

The $\mathrm{Nema}_{t,group}$ and $\mathrm{Nega}_{t,group}$ are the Nema and Nega of the feed and can be calculated using the composition of the feed ($\mathrm{x}_{t,j,group}$), the Nema (NemaC_j) and the Nega (NegaC_j) of the ingredients as well as Eqs.(D.31)-(D.32). Nega is the amount of energy from the diet consumed in the growth of the animal.

$$\mathrm{Nema_{t,group}}=\sum_{\mathrm{j}} \mathrm{x_{t,j,group}} \cdot \mathrm{NemaC_j} \ \forall t, group \tag{D.31}$$

$$\mathrm{Nega_{t,group}}=\sum_{\mathrm{j}} \mathrm{x_{t,j,group}} \cdot \mathrm{NegaC_j} \ \forall t, group \tag{D.32}$$

The energy available for livestock growth ($\mathrm{RE}_{t,group}$) is estimated by $\mathrm{DMI}_{t,group}$ (dry matter intake of feed), $\mathrm{Nega}_{t,group}$, and Im_t using Eq.(D.33). To determine the $\mathrm{DMI}_{t,group}$ corresponding to the formulated feed, Eq.(D.34) is used.

$$\begin{aligned}&\mathrm{RE_{t,group}(Mcal/day)=(DMI_{t,group}(kg/day)\text{-}}\\&\mathrm{Im_t(kg/day)) \cdot NEga_{t,group}(Mcal/day)} \ \forall t, group\end{aligned} \tag{D.33}$$

$$\mathrm{DMI}_{t,group} = \sum_j x_{t,j,group} \cdot DMIf_{j,t} \ \ \forall \mathrm{t,group} \tag{D.34}$$

D.1.4 *Supply of Nutrients and estimation of waste production*

Protein supplement

The animals can ingest proteins from two sources, feed ($\text{MPFeed}_{t,j,group}$) and bacterial activity $\text{MPBact}_{t,j,group}$). On the one hand, 80% of the protein available in feed (UIP) is digestible. Therefore, the $\text{MPFeed}_{t,j,group}$ is calculated by Eq.(D.35), with the information of crude protein (CP_j) of the ingredient 'j'. On the other hand, the microbial contribution is estimated using the microbial crude protein yield ($\text{MCP}_{t,j,group}$). This is determined from the total digestible nutrients TDN_j and the degradability yield of the neutral detergent fiber of the diet (eNDF) by Eq.(D.36). UIP_j,CP_j,TDN_j and eNDF_j can be consulted in nutritional tables in the literature (Council, 2000b) for the different type of ingredients. The assumption of 64% of ($\text{MCP}_{t,j,group}$) is true digestible protein ($\text{MPBact}_{t,j,group}$) is applied in Eq.(D.37). The total supplement ($\text{MPtot}_{t,j,group}$) will be the sum of the two contributions Eq.(D.38).

$$\begin{aligned}\text{MPfeed}_{t,j,group}(g/day) = {} & \frac{\text{UIP}_j(\%\text{CP})}{100} \cdot \frac{CP_j(\%DM)}{100} \cdot 0.8 \cdot \\ & \text{DMI}_{t,group}(\text{kg/day}) \cdot 1000(\text{kg/day}) \cdot \text{x}_{t,j}\end{aligned} \tag{D.35}$$

$$\text{MCP}_{\text{t,j},group}(\text{g/day}){=}0.13 \cdot \text{TDN}_\text{j}(\text{g/day})/100 \ \cdot eNDF_j \ \forall t,j,group \tag{D.36}$$

$$\text{MPBact}_{\text{t,j},group}(\text{g/day}){=}\text{MCP}_{\text{t,j,group}}(\text{g/day}) \cdot 0.64 \quad \forall t,j,group \tag{D.37}$$

$$\begin{aligned}&\text{MPtot}_{\text{t,j},group}(\text{g/day}){=}\text{MPbact}_{\text{t},group}(\text{g/day}) + \\ &\text{MPfeed}_{\text{t},group}(\text{g/day}) \ \forall t,j,group\end{aligned} \tag{D.38}$$

Supply of Energy and Protein

The energy can be supplied in the form of carbohydrates (CHO_j), non-fiber carbohydrates (NFC_j), sugar((CA_j)) and starch (CB1_j). Besides, it is also important to consider the parts of the food that are resistant to digestion, such as available fiber (CB2_j) and unavailable fiber (CC_j), to evaluate the composition of the residues. The nutritional information of the ingredients (crude protein (CP_j), neutral detergent insoluble protein in the crude protein (NDFIP_j), neutral detergent fiber (NDF_j), unavailable fiber (CC_j), nonstructural carbohydrate (STARCH_j), lignin (LIGNIN_j) can be consulted in the literature (Council, 2000b) and Table D.6, and used to estimate the previous sources of energy together with Eqs.(D.39)-(D.45).

$$\mathrm{CHO_j(\ \%\ DM)=100\text{-}CP_j(\ \%\ DM)\text{-}FAT_j(\ \%\ DM)\text{-}ASH_j(\ \%\ DM)}\ \forall j \tag{D.39}$$

$$\mathrm{CB2}_j(\%\mathrm{DM}) = \mathrm{NDF}_j(\%DM)- \tag{D.40}$$
$$(\mathrm{NDFIP}_j(\%\mathrm{DM})\cdot 0.01\cdot \mathrm{CP}_j(\%\mathrm{DM})\text{-}\mathrm{CC}_j(\%\mathrm{DM}))\forall j \tag{D.41}$$

$$\mathrm{NFC_j(\ \%\ DM)=CHO_j(\ \%\ DM)\text{-}CB2_j(\ \%\ DM)\text{-}CC_j(\ \%\ DM)}\ \forall j \tag{D.42}$$

$$\mathrm{CC_j(\ \%\ DM)=NDF_j(\ \%\ DM)\ \cdot\ 0.01\ \cdot LIGNIN_j(\ \%\ DM)\ \cdot\ 2.4}\ \forall j \tag{D.43}$$

$$\mathrm{CA_j(\ \%\ DM)=NDF_j(\ \%\ DM)\text{-}CB1_j(\ \%\ DM)}\ \forall j \tag{D.44}$$

$$\mathrm{CB1_j(\ \%\ DM)=STARCH_j(\ \%\ DM)\ \cdot\ NDF_j(\ \%\ DM)/100}\ \forall j \tag{D.45}$$

The proteins can be classified according to their degradation speed, depending on whether it is fast ($PB1_j$), medium ($PB2_j$) or slow ($PB3_j$). In addition of these, the crude protein (PC_j) must be considered. As in the case of carbohydrates, nutritional information (soluble protein ($SOLP_j$), neutral detergent insoluble protein ($NDFIP_j$), acid detergent insoluble protein ($ADFI_j$), crude protein that is non-protein nitrogen (PA_j),) (see Table D.6) is used to estimate the amount of protein present in the ingredients through Eqs.(D.46)-(D.49).

$$\mathrm{PB1_j(\ \%\ DM)=SOLP_j(\ \%\ CP)\ \cdot\ CP_j\ \cdot\ 0.01\text{-}PA_j(\ \%\ DM)}\ \forall j \tag{D.46}$$

$$\mathrm{PB3_j(\ \%\ DM)=(NDFIP_j(\ \%\ CP)\text{-}ADFIP_j(\ \%\ CP))\ \cdot\ CP_j\ \cdot 0.01}\ \forall j \tag{D.47}$$

$$\mathrm{PB2_j(\ \%\ DM)=CP_j(\ \%\ DM)\text{-}PA_j(\ \%\ DM)\text{-}}$$
$$\mathrm{PB1_j(\ \%\ DM)\text{-}PB3_j(\ \%\ DM)\text{-}PC_j(\ \%\ DM)}\ \forall j \tag{D.48}$$

$$\mathrm{PC_j(\ \%\ DM)=ADFIP_j(\ \%\ CP)\cdot\ CP_j(\ \%\ DM)\ \cdot\ 0.01}\ \forall j \tag{D.49}$$

Degradation of nutrients in the rumination phase

The degradation of nutrients is evaluated through the degradation ratio (Kp) and non-degradation (Kd). The estimation of Kp depends on whether the ingredient is forage Eq.(D.50) or concentrate Eq.(D.51). Kd is indicated in the nutritional information of the ingredients (Table D.6).

$$\text{Kp[forage]}=(0.388+(0.022\cdot \text{DMI}_{t,group}/\text{SBW}0.75)+2.0\cdot \text{FORAGE2})/100) \tag{D.50}$$

$$\text{Kp[conc]}=-0.424+(1.45\cdot \text{Kp[forage]}) \tag{D.51}$$

$\text{It}_{t,j,group}$ is the amount of each ingredient 'j' consumed in the TU 't' by the animal group 'group', which is calculated by Eq.(D.52) using the $\text{DMI}_{t,group}$ and the composition ($x_{t,j,group}$). Using Kp,Kd and $\text{It}_{t,j,group}$, the amount of degraded (Eqs.(D.53)-(D.57)) and non-degraded (Eqs.(D.58)-(D.61)) proteins of can be determine. On the one hand, $\text{RDPA}_{t,j,group}$, $\text{RDPB1}_{t,j,group}$, $\text{RDPB2}_{t,j,group}$, $\text{RDPB3}_{t,j,group}$ are the degraded amount of $\text{PA}_{t,j,group}$, $\text{PB1}_{t,j,group}$, $\text{PB2}_{t,j,group}$, $\text{PB3}_{t,j,group}$. On the other hand, $\text{REPB1}_{t,j,group}$, $\text{REPB2}_{t,j,group}$, $\text{RDPB3}_{t,j,group}$, $\text{REPC}_{t,j,group}$ are the non-degraded amount.

$$\text{It}_{\text{t,j},group}(\text{g/day})=\text{DMI}_{t,group}(\text{kg/day})\cdot x_{\text{t,j},group}\cdot 1000\text{g/kg}\ \forall t,j,group \tag{D.52}$$

$$\text{RDPA}_{\text{t,j},group}=\text{It}_{\text{t,j},group}\cdot \text{PA}_{\text{j}}\ \forall t,j,group \tag{D.53}$$

$$\text{RDPB1}_{\text{t,j},group}(\text{g/day})=\text{It}_{\text{t,j},group}(\text{g/day})\cdot \text{PB1}_{\text{j}}\cdot\left(\frac{\text{Kd}_{1\text{j}}}{(\text{Kd}_{1\text{j}}+\text{Kp}_{\text{j}}}\right)\ \forall t,j,group \tag{D.54}$$

$$\text{RDPB2}_{\text{t,j},group}(\text{g/day})=\text{It}_{\text{t,j},group}(\text{g/day})\cdot \text{PB2}_{\text{j}}\cdot\left(\frac{\text{Kd}_{2\text{j}}}{\text{Kd}_{2\text{j}}+\text{Kp}_{\text{j}}}\right)\ \forall t,j,group \tag{D.55}$$

$$\text{RDPB3}_{\text{t,j},group}(\text{g/day})=\text{It}_{\text{t,j},group}(\text{g/day})\cdot \text{PB3}_{\text{j}}\cdot\left(\frac{\text{Kd}_{3\text{j}}}{\text{Kd}_{3\text{j}}+\text{Kp}_{\text{j}}}\right)\ \forall t,j,group \tag{D.56}$$

$$\text{RDPEP}_{\text{t,j},group}(\text{g/day})=\text{RDPB1}_{\text{t,j},group}(\text{g/day})+\text{RDPB2}_{\text{t,j},group}(\text{g/day})$$
$$+\text{RDPB3}_{\text{t,j},group}(\text{g/day})\ \forall t,j,group \tag{D.57}$$

$$\mathrm{REPB1}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{PB1_j} \cdot \frac{\mathrm{Kp_j}}{\mathrm{Kd_{1j}} + \mathrm{Kp_j}} \; \forall t, j, group \tag{D.58}$$

$$\mathrm{REPB2}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{PB2_j} \cdot \frac{\mathrm{Kp_j}}{\mathrm{Kd_{2j}} + \mathrm{Kp_j}} \; \forall t, j, group \tag{D.59}$$

$$\mathrm{REPB3}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{PB3_j} \cdot \frac{\mathrm{Kp_j}}{\mathrm{Kd_{3j}} + \mathrm{Kp_j}} \; \forall t, j, group \tag{D.60}$$

$$\mathrm{REPC}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{PC_j} \; \forall t, j, group \tag{D.61}$$

$\mathrm{RDCA}_{t,j,group}$, $\mathrm{RDCB1}_{t,j,group}$ and $_{t,j,group}$ are the amount degraded of CA_j, $\mathrm{CB1}_j$ and $\mathrm{CB2}_j$, respectively. These variables are calculated by Eqs.(D.62)-(D.64). The non-degraded part ($\mathrm{RECA}_{t,j,group}$, $\mathrm{RECB1}_{t,j,group}$ and $\mathrm{RECB2}_{t,j,group}$) is estimated by Eqs.(D.65)-(D.67).

$$\mathrm{RDCA}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{CA_j} \cdot \left(\frac{\mathrm{Kd_{4j}}}{\mathrm{Kd_{4j}} + \mathrm{Kp_j}} \right) \; \forall t, j, group \tag{D.62}$$

$$\mathrm{RDCB1}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{CB1_j} \cdot \left(\frac{\mathrm{Kd_{5j}}}{\mathrm{Kd_{5j}} + \mathrm{Kp_j}} \right) \; \forall t, j, group \tag{D.63}$$

$$\mathrm{RDCB2}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{CB2_j} \cdot \left(\frac{\mathrm{Kd_{6j}}}{\mathrm{Kd_{6j}} + \mathrm{Kp_j}} \right) \; \forall t, j, group \tag{D.64}$$

$$\mathrm{RECA}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{CA_j} \cdot \left(\frac{\mathrm{Kp_j}}{\mathrm{Kd_{4j}} + \mathrm{Kp_j}} \right) \; \forall t, j, group \tag{D.65}$$

$$\mathrm{RECB1}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{It}_{\mathrm{t,j},group}(\mathrm{g/day}) \cdot \mathrm{CB1_j} \cdot \left(\frac{\mathrm{Kp_j}}{\mathrm{Kd_{5j}} + \mathrm{Kp_j}} \right) \; \forall t, j, group \tag{D.66}$$

$$\mathrm{RECB2}_{\mathrm{t,j,}group}(\mathrm{g/day}){=}\mathrm{It}_{\mathrm{t,j,}group}(\mathrm{g/day}) \cdot \mathrm{CB2_j} \cdot \left(\frac{\mathrm{Kp_j}}{\mathrm{Kd_{6j}}{+}\mathrm{Kp_j}}\right) \; \forall t, j, group \tag{D.67}$$

Calculation of Microbial Yield for carbohydrate fermenting

The bacterial decomposition yield of the fiber, sugar, and starch ($Y1_j$, $Y2_j$, $Y3_j$) are calculated by Eqs.(D.68)-(D.70). YG_1, YG_2 are set to 0.4 for both yields; and KM_1, K_2 are fixed at 0.05 and 0.15, respectively.

$$\frac{1}{\mathrm{Y1_j}}{=}\frac{\mathrm{KM_1}}{\mathrm{Kd_{6j}}}{+}\frac{1}{\mathrm{YG_1}} \; \forall j \tag{D.68}$$

$$\frac{1}{\mathrm{Y2_j}}{=}\frac{\mathrm{KM_2}}{\mathrm{Kd_{4j}}}{+}\frac{1}{\mathrm{YG_2}} \; \forall j \tag{D.69}$$

$$\frac{1}{\mathrm{Y3_j}}{=}\frac{\mathrm{KM_2}}{\mathrm{Kd_{5j}}}{+}\frac{1}{\mathrm{YG_2}} \; \forall j \tag{D.70}$$

It is possible to use these yields to estimate the two different sources of bacteria, fiber and non-fiber carbohydrate bacteria ($FCBACT_{t,j,group}$ and $NFCBACT_{t,j,group}$) by applying Eqs.(D.71) and (D.72), respectively.

$$\mathrm{FCBACT}_{\mathrm{t,j,}group}(\mathrm{g/day}){=}\mathrm{Y1_j} \cdot \mathrm{RDCB2}_{\mathrm{t,j,}group}(\mathrm{g/day}) \; \forall t, j, group \tag{D.71}$$

$$\begin{aligned}&\mathrm{NFCBACT}_{\mathrm{t,j,}group}(\mathrm{g/day}){=}(\mathrm{Y2_j} \cdot \mathrm{RDCA}_{\mathrm{t,j,}group}(\mathrm{g/day})){+}\\&(\mathrm{Y3_j} \cdot \mathrm{RDCB1}_{\mathrm{t,j,}group}(\mathrm{g/day})) \; \forall t, j, group\end{aligned} \tag{D.72}$$

The sum of these variables (Eq.(D.73)) is the amount of bacteria generated ($BACT_{t,j,group}$).

$$\mathrm{BACT}_{\mathrm{t,j,}group}{=}\mathrm{NFCBACT}_{\mathrm{t,j,}group}{+}\mathrm{FCBACT}_{\mathrm{t,j,}group} \; \forall t, j, group \tag{D.73}$$

10% of the bacteria, the bacteria fiber carbohydrate, and the bacteria non-fiber carbohydrate is nitrogen ($BACTN_{t,j,group}$, $FCBACTN_{t,j,group}$, $NFCBACTN_{t,j,group}$, respectively). These variables are calculated by Eqs.(D.74)-(D.76).

$$\mathrm{BACTN}_{\mathrm{t,j,}group}(\mathrm{g/day}){=}0.1 \cdot \mathrm{BACT}_{\mathrm{t,j,}group}(\mathrm{g/day}) \; \forall t, j, group \tag{D.74}$$

$$\mathrm{NFCBACTN}_{\mathrm{t,j,}group}(\mathrm{g/day}){=}0.1 \cdot \mathrm{NFCBACT}_{\mathrm{t,j,}group}(\mathrm{g/day}) \; \forall t, j, group \tag{D.75}$$

$$\text{FCBACTN}_{\text{t,j},group}(\text{g/day})\text{=0.1} \cdot \text{FCBACT}_{\text{t,j}}(\text{g/day}) \ \forall t, j, group \tag{D.76}$$

On the hand, the bacterial peptide ($PEPUP_{t,j,group}$) is obtained from the degradation of proteins in the rumination phase ($REPEP_{t,j,group}$) and is calculated by Eq.(D.77). On the other hand, Eq.(D.78) calculates of the nitrogen of the bacterial peptide ($PEPUPN_{t,j,group}$).

$$\text{PEPUP}_{\text{t,j},group}(\text{g/day})\text{=RDPEP}_{\text{t,j},group}(\text{g/day}) \ \forall t, j, group \tag{D.77}$$

$$\text{PEPUPN}_{\text{t,j},group}(\text{g/day})\text{=PEPUP}_{\text{t,j},group}(\text{g/day})/6.25 \ \forall t, j, group \tag{D.78}$$

The excess nitrogen of the bacterial rumen ($EN_{t,group}$) is given by Eq.(D.79). The bacterial nitrogen balance ($BACTNBAL_{t,j,group}$) is estimated by Eq.(D.80) and the peptide balance ($PEPBAL_{t,j,group}$) is shown in Eq.(D.82). U is the ruminant nitrogen usage and is predicted by Eq.(D.83).

$$\text{EN}_{\text{t},group}(\text{g/day})\text{=}\sum_{\text{j}} \text{PEPUPN}_{\text{t,j},group}(\text{g/day})\text{+}\frac{\sum_{\text{j}} \text{RDPA}_{\text{t,j},group}(\text{g/day})}{6.25}+ \left(\frac{\sum_{\text{j}} \text{MPa}_{\text{t,j}}(\text{g/day})\text{-MPreq}_{\text{t}}(\text{g/day})}{6.25}\right)\text{-}\sum_{\text{j}} \text{BACTN}_{\text{t,j},group}(\text{g/day}) \ \forall t, group \tag{D.79}$$

$$\text{BACTNBAL}_{\text{t,j},group}(\text{g/day})\text{=(((}\frac{\text{PEPUP}_{\text{t,j},group}(\text{g/day})\text{+RDPA}_{\text{t,j},group}(\text{g/day}))}{6.25}\text{)+}$$
$$\text{U}_{\text{j}}(\text{g/day}))\text{-BACTN}_{\text{t,j},group}(\text{g/day}) \ \forall t, j, group \tag{D.80}$$

$$\text{PEPBAL}_{\text{t,j},group}(\text{g/day})\text{=}\frac{\text{PEPUP}_{\text{t,j},group}(\text{g/day})}{6.25}\text{-(2/3)} \tag{D.81}$$
$$\cdot \text{NFCBACTN}_{\text{t,j},group}(\text{g/day}) \ \forall t, j, group \tag{D.82}$$

$$\text{U}_{\text{j}}\text{=121.7-12.01} \cdot \text{CP}_{\text{j}}\text{+0.3235} \cdot \text{CP}_{\text{j}}^{2} \ \forall j \tag{D.83}$$

The content of carbohydrates ($REBCHO_{t,j,group}$), fat ($REBFAT_{t,j,group}$), true protein ($REBTP_{t,j,group}$), bacterial cell wall protein ($REBCW_{t,j,group}$), bacterial nucleic acids ($REBNA_{t,j,group}$) and ashes ($REBASH_{t,j,group}$) in bacterial can be determined by Eqs.(D.84)-(D.89).

$$\text{REBCHO}_{\text{t,j},group}(\text{g/day})\text{=0.21} \cdot \text{BACT}_{\text{t,j},group}(\text{g/day}) \ \forall t, j, group \tag{D.84}$$

$$\mathrm{REBFAT}_{\mathrm{t,j},group}(\mathrm{g/day}) = 0.12 \cdot \mathrm{BACT}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.85}$$

$$\mathrm{REBTP}_{\mathrm{t,j},group}(\mathrm{g/day}) = 0.6 \cdot 0.625 \cdot \mathrm{BACT}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.86}$$

$$\mathrm{REBCW}_{\mathrm{t,j},group}(\mathrm{g/day}) = 0.25 \cdot 0.625 \cdot \mathrm{BACT}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.87}$$

$$\mathrm{REBNA}_{\mathrm{t,j},group}(\mathrm{g/day}) = 0.15 \cdot 0.625 \cdot \mathrm{BACT}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.88}$$

$$\mathrm{REBASH}_{\mathrm{t,j},group}(\mathrm{g/day}) = 0.044 \cdot \mathrm{BACT}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.89}$$

Intestinal digestion process.
The amount of fats, carbohydrates, and proteins, that are not digested in the rumination phase, are assimilated in the intestinal digestion process. In the case of proteins, the amount of digestible of rapidly degraded protein ($\mathrm{DIGPB1}_{t,j,group}$), intermediately degraded protein($\mathrm{DIGPB2}_{t,j,group}$), slowly degraded protein ($\mathrm{DIGPB3}_{t,j,group}$) are given by Eqs.(D.90)-(D.92). The sum of these variables ($\mathrm{DIGFP}_{t,j,group}$) is calculated by Eq.(D.93).

$$\mathrm{DIGPB1}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{REPB1}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.90}$$

$$\mathrm{DIGPB2}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{REPB2}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.91}$$

$$\mathrm{DIGPB3}_{\mathrm{t,j},group}(\mathrm{g/day}) = 0.8 \cdot \mathrm{REPB3}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.92}$$

$$\mathrm{DIGFP}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{DIGPB1}_{\mathrm{t,j},group}(\mathrm{g/day}) + \mathrm{DIGPB2}_{\mathrm{t,j},group}(\mathrm{g/day}) + \mathrm{DIGPB3}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.93}$$

There are two sources of bacterial protein, the digestible bacterial true protein ($\mathrm{DIGBTP}_{t,j,group}$) and the digestible bacterial nucleic acids ($\mathrm{DIGBNA}_{t,j,group}$), which are estimated by Eqs.(D.94) and (D.95), respectively.

$$\mathrm{DIGBTP}_{\mathrm{t,j},group}(\mathrm{g/day}) = \mathrm{REBTP}_{\mathrm{t,j},group}(\mathrm{g/day}) \ \forall t, j, group \tag{D.94}$$

$$\text{DIGBNA}_{\text{t,j},group}(\text{g/day})\text{=REBNA}_{\text{t,j},group}(\text{g/day})\ \forall t,j,group \tag{D.95}$$

Therefore, the total amount of protein ($\text{DIGP}_{t,j,group}$) is shown in Eq.(D.96).

$$\text{DIGP}_{\text{t,j},group}\text{=DIGFP}_{\text{t,j},group}\text{+DIGBTP}_{\text{t,j},group}\text{+DIGBNA}_{\text{t,j},group}\ \forall t,j,group \tag{D.96}$$

Regarding digested carbohydrates, two sources are considered, feed (($\text{DIGFC}_{t,j,group}$)) and bacterias ($\text{DIGBC}_{t,j,group}$) and are given by Eqs.(D.97)-(D.98). The stdig is the postruminal starch digestibility. This value can be consulted in the literature (Council, 2000b).

$$\begin{aligned}&\text{DIGFC}_{\text{t,j},group}(\text{g/day})\text{=RECA}_{\text{t,j},group}(\text{g/day})\text{+stdig}\cdot\text{RECB1}_{\text{t,j},group}(\text{g/day})\\&+0.2\cdot\text{RECB2}_{\text{t,j},group}(\text{g/day})\ \forall t,j,group\end{aligned} \tag{D.97}$$

$$\text{DIGBC}_{\text{t,j},group}(\text{g/day})\text{=0.95}\cdot\text{REBCHO}_{\text{t,j},group}(\text{g/day})\ \forall t,j,group \tag{D.98}$$

The total amount of digested carbohydrates ($\text{DIGC}_{t,j,group}$) is shown by Eq.(D.99).

$$\begin{aligned}&DIGC_{t,j,group}(g/day) = DIGFC_{t,j,group}(g/day)+\\&DIGB_{t,j,group}(g/day)\forall t,j,group\end{aligned} \tag{D.99}$$

Lastly, the fat not digested in the rumination phase, so it passes in its entirety to the intestine ($\text{REFAT}_{t,j,group}$), as indicated in Eq.(D.100). The digested fat in the intestines has two sources, the feed ($\text{DIGFF}_{t,j,group}$) and the bacteria ($\text{DIFBF}_{t,j,group}$). The estimation of both sources is indicated in Eqs.(D.101) and (D.102) and , while the sum ($\text{DIGF}_{t,j,group}$) is calculated by Eq.(D.103).

$$\text{REFAT}_{\text{t,j,group}}(\text{g/day})\text{=It}_{\text{t,j,group}}(\text{g/day})\cdot\text{FAT}_{\text{t,j}}\ \forall t,j \tag{D.100}$$

$$\text{DIGFF}_{\text{t,j},group}(\text{g/day})\text{=0.95}\cdot\text{REFAT}_{\text{t,j},group}(\text{g/day})\ \forall t,j,group \tag{D.101}$$

$$\text{DIGBF}_{\text{t,j},group}(\text{g/day})\text{=0.95}\cdot\text{REBFAT}_{\text{t,j},group}(\text{g/day})\ \forall t,j,group \tag{D.102}$$

$$\text{DIGF}_{\text{t,j},group}(\text{g/day})\text{=DIGFF}_{\text{t,j},group}(\text{g/day})\text{+DIGBF}_{\text{t,j},group}(\text{g/day}) \ \forall t, j, group \tag{D.103}$$

Composition of waste.

The composition of the waste expelled by cattle can be estimated using the calculations of the previous section. The sum of the undigested proteins ($\text{FEFP}_{t,j,group}$) is composed of the undigested part of the proteins B3 ($\text{FEPB3}_{t,j,group}$) and C ($\text{FEPC}_{t,j,group}$) and are calculated in Eqs.(D.104)-(D.106).

$$\text{FEFP}_{\text{t},group}(\text{g/day})\text{=FEPB3}_{\text{t},group}(\text{g/day})\text{+FEPC}_{\text{t},group}(\text{g/day}) \ \forall t, group \tag{D.104}$$

$$\text{FEPB3}_{\text{t},group}(\text{g/day})\text{=}\sum_j \Big((\text{1-0.8}) \cdot \text{REPB3}_{\text{t,j},group}(\text{g/day})\Big) \ \forall t, group \tag{D.105}$$

$$\text{FEPC}_{\text{t},group}(\text{g/day})\text{=}\sum_j (\text{REPC}_{\text{t,j},group}(\text{g/day})) \ \forall t, group \tag{D.106}$$

The sum of carbohydrates ($\text{FEFC}_{t,j,group}$) is formed by starch ($\text{FECB1}_{t,j,group}$), available fiber ($\text{FECB2}_{t,j,group}$), unavailable fiber ($\text{FECC}_{t,j,group}$). These variables are calculated using Eqs.(D.107)-(D.110).

$$\begin{aligned}&\text{FEFC}_{\text{t,j},group}(\text{g/day})\text{=}\sum_j (\text{FECB1}_{\text{t,j},group}(\text{g/day})\text{+}\\&\text{FECB2}_{\text{t,j},group}(\text{g/day})\text{+FECC}_{\text{t,j},group}(\text{g/day})) \ \forall t, j, group\end{aligned} \tag{D.107}$$

$$\text{FECB1}_{\text{t},group}(\text{g/day})\text{=}\sum_j \big((\text{1-stdig}) \cdot \text{RECB1}_{\text{t,j},group}(\text{g/day})\big) \ \forall t, group \tag{D.108}$$

$$\text{FECB2}_{\text{t},group}(\text{g/day})\text{=}\sum_j \big((\text{1-0.2}) \cdot \text{RECB2}_{\text{t,j},group}(\text{g/day})\big) \ \forall t, group \tag{D.109}$$

$$\text{FECC}_{\text{t},group}(\text{g/day})\text{=}\sum_j \big(\text{RECC}_{\text{t,j},group}(\text{g/day})\big) \ \forall t, group \tag{D.110}$$

Fat only has one source ($FEFF_{j,group}$) and is estimated by Eq.(D.111). The ashes are not digested and therefore, they are expelled with feces ($FEFA j, group$) and are quantified by Eq.(D.112).

$$\mathrm{FEFF}_{t,group}(\mathrm{g/day}) = \sum_j \left(\mathrm{REFAT}_{t,j,group}(\mathrm{g/day}) \cdot (1\text{-}0.95)\right) \; \forall t, group \tag{D.111}$$

$$\mathrm{FEFA}_{t,group}(\mathrm{g/day}) = \sum_j \left(\mathrm{It}_{t,j,group}(\mathrm{g/day}) \cdot \mathrm{ASH}_j \cdot (1\text{-}0.5)\right) \; \forall t, group \tag{D.112}$$

The total amount of proteins, carbohydrates and fats that come from bacteria and are present in the feces can be determined through the bacterial composition of feces. On the one hand, the amount of fecal bacterial cell wall protein ($FEBCW_{t,j,group}$) and the amount of fecal bacterial protein ($FEBCP_{t,j,group}$) are estimated by Eqs.(D.113) and (D.114). On the other hand, the amount of bacterial carbohydrate ($FEBC_{t,j,group}$), fat ($FEBF_{t,j,group}$) and ash ($FEBASH_{t,j,group}$) are calculated by Eqs.(D.115)-(D.117). The sum of all the amount of bacteria present in the feces ($FEBACT_{t,j,group}$) is given by Eq.(D.118).

$$\mathrm{FEBCW}_{t,group}(\mathrm{g/day}) = \sum_j \left(\mathrm{REBCW}_{t,j,group}(\mathrm{g/day})\right) \; \forall t, group \tag{D.113}$$

$$\mathrm{FEBCP}_{t,group}(\mathrm{g/day}) = \mathrm{FEBCW}_{t,group}(\mathrm{g/day}) \; \forall t, group \tag{D.114}$$

$$\mathrm{FEBC}_{t,group}(\mathrm{g/day}) = \sum_j (1\text{-}0.95) \cdot \mathrm{REBCHO}_{t,j,group}(\mathrm{g/day}) \; \forall t, group \tag{D.115}$$

$$\mathrm{FEBF}_{t,group}(\mathrm{g/day}) = \sum_j \left((1\text{-}0.95) \cdot \mathrm{REBFAT}_{t,j,group}(\mathrm{g/day})\ \right) \quad \forall t, group \tag{D.116}$$

$$\mathrm{FEBASH}_{t,group}(\mathrm{g/day}) = \sum_j \left((1\text{-}0.5) \cdot \mathrm{REBASH}_{t,j,group}(\mathrm{g/day})\right) \; \forall t, group \tag{D.117}$$

$$\text{FEBACT}_{t,group}\text{(g/day)=FEBCW}_{t,group}\text{(g/day)+FEBCP}_{t,group}\text{(g/day)} \\ \text{+FEBC}_{t,group}\text{(g/day)+FEBF}_{t,group}\text{(g/day)+FEBASH}_{t,group}\text{(g/day)}\ \forall t, group \tag{D.118}$$

The indigestible dry matter (IDM) is estimated by Eq.(D.119). There is a certain amount of proteins ($FEENGP_{t,j,group}$), fats ($FEENGF_{t,j,group}$) and ashes ($FEENGA_{t,j,group}$) that are endogenously generated. This amount is estimated by Eqs.(D.120)-(D.122).

$$\text{IDM}_{t,j,group}\text{(kg/day)=(100-TDN}_j\text{)/100} \cdot \text{DMIf}_{t,j} \cdot \text{x}_{t,j,group}\quad \forall t, j, group \tag{D.119}$$

$$\text{FEENGP}_{t,group}\text{(g/day)=}\sum_j 0.09 \cdot \text{IDM}_{t,j,group}\text{(kg/day)} \cdot 1000\text{g/kg}\ \forall t, j, group \tag{D.120}$$

$$\text{FEENGF}_{t,group}\text{(g/day)=}\sum_j 0.0119 \cdot \text{DMI}_{t,j,group}\text{(g/day)} \cdot 1000\text{g/kg}\ \forall t, j, group \tag{D.121}$$

$$\text{FEENGA}_{t,group}\text{(g/day)=}\sum_j \left(0.017 \cdot \text{DMI}_{t,j,group}\text{(g/day)} \cdot 1000\text{g/kg}\right)\ \forall t, group \tag{D.122}$$

Summing all protein sources ($FEPROT_{t,group}$) in Eq.(D.123), carbohydrates ($FECHO_{t,group}$) in Eq.(D.124), fats ($FEFAT_{t,group}$) in Eq.(D.125) ,and ashes ($FEASH_{t,group}$) in Eq.(D.126).

$$\text{FEPROT}_{t,group}\text{(g/day)=FEFP}_{t,group}\text{(g/day)+} \\ \text{FEBCP}_{t,group}\text{(g/day)+FEENGP}_{t,group}\text{(g/day)}\ \forall t, group \tag{D.123}$$

$$\text{FECHO}_{t,j,group}\text{(g/day)=FEFC}_{t,group}\text{(g/day)+FEBC}_{t,group}\text{(g/day)}\ \forall t, group \tag{D.124}$$

$$\text{FEFAT}_{t,group}\text{(g/day)=FEBF}_{t,group}\text{(g/day)+FEFF}_{t,group}\text{(g/day)+} \\ \text{FEENGF}_{t,group}\text{(g/day)}\ \forall t, group \tag{D.125}$$

$$\text{FEASH}_{t,group}\text{(g/day)=FEFA}_{t,group}\text{(g/day)+} \\ \text{FEBASH}_{t,group}\text{(g/day)+FEENGA}_{t,group}\text{(g/day)}\ \forall t, group \tag{D.126}$$

All the equations of the model are adapted to be integrated into GAMS. Eqs.(D.127)-(D.129) are added to optimization model to calculate the total amount of protein ($FEPROTT_{t,group}$), fat ($FEFATT_{t,group}$) and carbohydrate ($FECHOT_{t,group}$) .Where $Nanimals_{t,group}$ is the total number of animals of each group.

$$\mathrm{FEPROTT}_{\mathrm{t},group}(\mathrm{g/day})=\mathrm{FEPROT}_{\mathrm{t},group}(\mathrm{g/day}) \cdot \mathrm{Nanimals}_{\mathrm{t,group}} \ \forall t, group \tag{D.127}$$

$$\mathrm{FEFATT}_{\mathrm{t},group}(\mathrm{g/day})=\mathrm{FEFAT}_{\mathrm{t},group}(\mathrm{g/day}) \cdot \mathrm{Nanimals}_{\mathrm{t,group}} \ \forall t, group \tag{D.128}$$

$$\mathrm{FECHOT}_{\mathrm{t},group}(\mathrm{g/day})=\mathrm{FECHO}_{\mathrm{t},group}(\mathrm{g/day}) \cdot \mathrm{Nanimals}_{\mathrm{t,group}} \ \forall t, group \tag{D.129}$$

D.2 WASTE TREATMENT AND NUTRIENT RECOVERED SYSTEMS

Anaerobic digestion is the technology used for the neutralization of waste and the production of biogas and digestate. Material balances are applied to determine the amounts of the reaction products (bacteria ($mbat_t$), methane ($mCH4_t$), carbon dioxide ($mCO2_t$), ammonia ($mNH3_t$) and water ($mH2O_t$)), using stoichiometric coefficients and empirical yields from literature (Taifouris & Martín, 2018) (Eqs.(D.130)-(D.134)).

$$\mathrm{mbat}_t\text{=}(0.1857 \cdot \mathrm{mlipids_t} + 0.1508 \cdot mch_t + 0.1241 \cdot mprot_t) \cdot xbio \ \forall t \tag{D.130}$$

$$\mathrm{mch4}_t\text{=}((0.6588 \cdot mlipid_t + 0.2433 \cdot mch_t + 0.2383 \cdot mprot_t) \cdot xbio \ \forall t \tag{D.131}$$

$$\mathrm{mCO2}_t\text{=}(0.6644 \cdot \mathrm{mlipids_t}\text{+}0.6675 \cdot \mathrm{mch_t}\text{+}0.6822 \cdot \mathrm{mpro_t}) \cdot xbio \ \forall t \tag{D.132}$$

$$\mathrm{m}NH3_t = (-0.0280 \cdot mlipid_t - 0.0227 \cdot mch_t + 0.1647 \cdot mprot_t) \cdot xbio \ \forall t \tag{D.133}$$

$$\mathrm{mH2O_t}\text{=(-}0.481 \cdot \mathrm{mlipid_t}\text{-}0.039 \cdot \mathrm{mch_t} - 0.2047 \cdot mprot_t) \cdot xbio \ \forall t \tag{D.134}$$

Where xbio is the biodegradability of the substrate and whose value is set at 0.51 (Kafle & Chen, 2016) for cattle manure. $mlipids_t$, mch_t, $mprot_t$ are the mass of lipids, carbohydrates, proteins, respectively. This variables are calculated by Eqs.(D.135)-(D.137). It is necessary to calculate the amount of lignin and ash ($mlign_t$ and $mash_t$) to know the total amount of digestate. Therefore, the Eqs.(D.138) and (D.139) are add to model.

$$\mathrm{mlipids}_t = \sum_{group} \mathrm{FEFATT}_{\mathrm{t,j},group} \; \forall t \tag{D.135}$$

$$\mathrm{mch}_t = \sum_{group} \mathrm{FECHOT}_{\mathrm{t,j},group} \; \forall t \tag{D.136}$$

$$\mathrm{mprots}_t = \sum_{group} \mathrm{FEPROTT}_{\mathrm{t,j},group} \; \forall t \tag{D.137}$$

$$\mathrm{mlign}_t = \sum_{group} FELIGT_{t,group} \; \forall t \tag{D.138}$$

$$\mathrm{mash}_t = \sum_{group} FEASH_{t,group} \; \forall t \tag{D.139}$$

Different technologies for the purification of biogas can be combined to obtain energy through its combustion, such as a bed of Fe_2O_3 to remove the H_2S, a scrubber to reduce ammonia content down to 5%, and a pressure swing adsorption system to remove the water, 95% of the CO_2 and the rest of the ammonia(León & Martín, 2016). The liquid and solid effluents are separated using a decanter centrifuge. The solid retained 25% of ammonia and this is lost in the storage. The NH_3 is recovered (Nrec) by transmembrane chemisorption, that has a yield of 58%. The rest of nutrient (Prec and Krec) are totally recovered. The mass balance of the recovered nutrient is estimated by Eqs.(D.140)-(D.146).

$$\mathrm{N}_{\mathrm{rec}} = \sum_t 0.582 \cdot \mathrm{NH}_{3_{1_t}} \tag{D.140}$$

$$\mathrm{P}_{\mathrm{rec}} = \sum_t \mathrm{Psup}_{\mathrm{feed}_t} + \mathrm{Psup}_{\mathrm{supp}_t} - \mathrm{P}_{\mathrm{nd}_t} \tag{D.141}$$

$$\mathrm{Psup}_{\mathrm{feed}_t} = \frac{\mathrm{DMIf}_t \cdot \mathrm{x}_{t,j,group} \cdot \mathrm{phosphoreo_j} \cdot \mathrm{DM_j}}{10000} \; \forall t \tag{D.142}$$

$$\mathrm{P_{nd}} = \frac{0.016 \cdot \mathrm{SBW}}{0.68} + \frac{\mathrm{Npg} \cdot 0.045}{0.68} + \frac{\mathrm{Yn} \cdot 0.95}{0.68} \tag{D.143}$$

$$\mathrm{K_{rec}} = \sum_t \mathrm{Ksup_{feed_t}} - \mathrm{K_{nd_t}} \tag{D.144}$$

$$\mathrm{Ksup_{feed_t}} = x_{t,j,grupo} \cdot DMIf_t \cdot potassiumo_j \; \forall t \tag{D.145}$$

$$\mathrm{K_{nd_t}} = \frac{0.6 * DMI_t}{100} \; \forall t \tag{D.146}$$

$NH3l_t$ is the ammonia of the liquid phase of the bioreactor. Knd and Pnd are the minerals necessary for the animals, while $Ksupfeed_t$ and $Psupfeed_t$ are the minerals supplied with feed. Lastly, Psupsupp is the phosphorus supplied by the supplement.

D.3 FERTILIZER FORMULATION

The amount of the necessary mineral fertilizer, which must be added together with organic fertilizer, is estimated by Eqs.(D.147)-(D.149).

$$\mathrm{N_{mine}} \cdot \mathrm{x_N} = \mathrm{N_{nd}} - \mathrm{N_{rec}} \tag{D.147}$$

$$\mathrm{P_{mine}} \cdot \mathrm{x_P} = \mathrm{P_{nd}} - \mathrm{P_{rec}} \tag{D.148}$$

$$\mathrm{K_{mine}} \cdot \mathrm{x_K} = \mathrm{K_{nd}} - \mathrm{K_{rec}} \tag{D.149}$$

Where x_N, x_P, and x_K (0.34, 0.2, and 0.5) (Agrifeed, 2021) are the composition of nitrogen, phosphorus, and potassium in the mineral fertilizer, respectively. N_{mine} is the amount of ammonium nitrate used to supply the amount of nitrogen to the system while P_{mine} is the amount of simple perphosphate. K_{mine} is the amount of potassium sulfate.

D.4 ENVIRONMENTAL IMPACT INDEX

The value of the indexes considered (global warming potential (GWP), eutrophication potential (EUp) for the fertilizer used are shown in the Table D.2 .

Table D.2: .- Environmental indexes of mineral nutrients (Nemecek & Erzinger, 2003; Daccache et al., 2014; Skowrońska & Filipek, 2014; Serenella et al., 2018)

	Ammonium Nitrate	Single superphosphate	Potassium sulphate	Weight
GWP (tCO2-Eq/tfertilizer)	0.93	0.12	1.02	0.65
EUp(kgPO4-3eq/tfertilizer)	0.17	0.11	0.18	0.09

In addition to the indexes shown in the table above, the water footprint of crops and animals is included. The total water footprint is made up of the rainwater consumed (green water footprint) and the water supplied artificially (blue water footprint). The water used for waste treatment (grey water footprint) is not used because only a single technology is considered. The green water footprint of each crop can be found in Table D.3 . The water consumption of the animals is 3.5 liters for calves, 25 liters for yearlings, and 70 liters for cows and bulls (Lanuza, 2006; Duarte, 2011). The weight of this index in the composite index will be 26%.

Table D.3: .-Green water footprint of crops (Kannan et al., 2017)

Crops	**l/kg**
Sorgo	969
Corn Forage	532
Alfalfa	532
Barley	816
Vetch	532
Barley Forage	532
Wheat	730
Oat	870
corn	477
Rye	870

While the upper and the lower limits of these indexes for a starting point of 1000 animals are shown int the Table D.4.

Table D.4: .-Maximum and minimum values of the environmental indexes considered

	Min	Max
GWP ($t_{CO2-Eq}/t_{Nutrient}$)	14142.45	75399.78
Eutrophication potential($kg_{PO4-3eq}/t_{Nutrient}$)	3485.36	17172.72
Water footprint(m^3)	71118000	1.5671E8
CI	0	1

D.5 CROPS MANAGEMENT

The considered ingredients, as well as their production cost, nutrient requirements, prices, and water consumption as a irrigated crop are shown in the Table D.5. On the one hand, the production yields of each location for each crop can be seen in Tables D.12-D.13. On the other hand, the nutritional characteristics of the crops can be seen in the Table D.6. In this section, the location dimension is introduced since all variables affecting location are related to crops management. To determine the required amount of crop per year, it is necessary to evaluate the total amount per year consumed of each ingredient by each type of animal in each group, i.e., calves ($\text{TotalAmountCA}_{j,year,group}$), yearling($\text{TotalAmountY}_{j,year,group}$) and cow($\text{TotalAmountCO}_{j,year,group}$). These amount are estimated by Eqs.(D.150)-(D.152)

Table D.5: .-Production cost and fertilizer consumption of the considered crops (Bellido, 2010, 2013; El confidencial químico, 2016; Ministerio de Agricultura pesca y alimentación, 2019a; Lonja de León, 2020; Ministerio de agricultura pesca y alimentación, 2020; Echemi, 2021)

Crop	Crop production cost(€/kg)	Necessary nutrients (kg/ha)	Price (€/kg)	Water consumption (Irrigated crop)
Alfalfa	0.029112	30N/240P/300K	0.168	3528
Vetch, Hay	0.058224	100N/85P/130K	0.111	3528
Barley, Forage	0.058224	100N/85P/130K	0.090	839
Barley, Straw	0.0612122	50N/22P/100K	0.030	1306
Wheat, Straw	0.0411382	102N/41P/95K	0.030	2241
Corn Forage	0.019408	190N/120P/220K	0.090	5349
Oat hay	0.0864996	44N/19P/39K	0.173	4000
Corn Grain	0.0231775	259N/120P/240K	0.233	5578
Sorgo	0.058224	95N/85P/110K	0.171	2000
Barley Grain	0.0612122	50N/22P/100K	0.190	1306
Wheat Grain	0.0411382	102N/41P/95K	0.215	2241
Rye grain	0.0796980	33N/22P/32K	0.172	-
Calcium Carbonate	-	-	0.065	-
Mono-Sodium Phosphate	-	-	1.2	-

Table D.6: .-Nutritional and energy characteristic of the considered ingredients (Council, 2000b)

Crop	Alfalfa	Vecth	Barley Forage	Barley Straw	Corn Forage	Wheat Straw	Oat hay	Corn Grain	Barley GRain	Wheat Grain	Rye GRain	Sorgo
Type	**Forage**							**Concentrate**				
DM(%AF)	38.0	89	91	91	25	89	92.2	88	92	90	88	70
NDF(%DM)	47.00	48	72.5	72.5	60	78.9	74.4	9	28	9.7	19	23
Lignin(%NDF)	23.40	16.67	13.75	13.75	5	16.47	20	2.22	20.8	4.29	5.3	6.09
eNDF(%NDF)	82	92	100	100	81	98	98	0	36	2.6	34	34
TDN(%DM)	58.0	57	40	40	65	41.0	45	88	75	85	84	88
ME(Mcal/kg)	2.10	2.06	1.45	1.45	2.35	1.48	1.63	3.18	2.71	3.07	3.04	2.75
NEm(Mcal/kg)	1.24	1.21	0.6	0.60	1.47	0.64	0.79	2.18	1.79	2.09	2.06	1.82
Neg(Mcal/kg)	0.68	0.64	0.08	0.08	0.88	0.11	0.25	1.5	1.16	1.42	1.4	1.19
CP(%DM)	17	20.8	4.4	4.4	9	3.5	4.4	9.8	48.9	11.3	13.8	12.40
DIP(%CP)	91.0	86	30	30	78	31	55	57.4	57	74	79	50.8
solCP(%CP)	45.0	28	20	20	45	20	20	11	20	30	53	12.0
NPN(%SolCP)	100.00	96	95	95	100	95	95	73	40	73	19	33
NDFIP(%CP)	32.00	25.2	75	75	16	75	75	15	10	4	7	10
ADPIP(%CP)	18.00	14	65	65	4.5	65	65	5	8	2	4	5
Starch(%NSC)	89	60	100	100	80	100	5	90	90	90	90	90
Fat(%DM)	3.10	3	1.9	1.9	3.1	2	2.2	4.3	1.7	1.9	1.7	3.10
Ash(%DM)	9.00	7	7.5	7.5	11	7.7	7.8	1.6	7	2	2	2
KCA (hr-1)	10	250	250	250	10	250	250	250	300	300	300	150
KC1(hr-1)	25	30	30	30	30	50	30	25	25	40	40	10
KC2(hr-1)	5.5	5.S	3	3.0	4	3	3	6	6	6	8	5.0
KB1(hr-1)	150	150	135	135	300	135	135	135	175	300	300	135
KB2(hr-1)	11	9	11	11	10	11	11	10	8	12	12	6
KB3(hr-1)	1.75	1.25	0.09	0.09	0.2	0.09	0.09	0.1	0.25	0.35	0.35	0.12
Ca(%DM)	1.74	1.36	0.3	0.3	0.52	0.17	0.23	0.03	0.16	0.07	0.07	0.05
P(%DM)	0.27	0.34	0.07	0.07	0.31	0.05	0.06	0.31	0.76	0.33	0.36	0.34
Mg(%DM)	0.33	0.27	0.23	0.23	0.31	0.12	0.17	0.11	0.35	0	0.14	0.14
CI(%DM)	0.41	0	0.67	0.67	0	0.32	0.78	0.06	0	11	0.03	0.09
K(%DM)	2.35	2.12	2.37	2.37	1.64	1.41	2.53	0.33	1.22	0	0.52	0.47
Na(%DM)	0.16	0.52	0.14	0.14	0	0.14	0.42	0.01	0.03	0.43	0.03	0.04
S(%DM)	0.31	0.15	0.17	0.17	0	0.19	0.22	0.14	0.26	0.02	0.17	0.12

$$TotalAmountCA_{\text{j,year,group}} = \sum_{t=1TU+Destemporal(group)}^{t=12TU+Destemporal(group)} \text{DMI}_t \cdot$$
$$x_{\text{t,j,gruop}} \cdot \text{Ncalves}_{group} \; \forall j, year, group \tag{D.150}$$

$$\text{TotalAmountY}_{\text{j,year,group}} = \sum_{t=5TU+Destemporal(group)}^{t=21TU+Destemporal(group)} \text{DMI}_t \cdot$$
$$x_{\text{t,j,gruop}} \cdot \text{Nyearling}_{\text{group}} \forall j, year, group \tag{D.151}$$

$$\text{TotalAmountCO}_{\text{j,year,group}} = \sum_{t=22TU+Destemporal(group)}^{t=71TU+Destemporal(group)} \text{DMI}_t \cdot x_{\text{t,j,gruop}}$$
$$\cdot \text{Ncows}_{group} \forall j, year, group \tag{D.152}$$

The sum of the amount of each crop 'j', in each location 'l', and each year 'year' ($\text{Amount}_{l,j,year}$) must be equal to the total amount demanded by the animals in a year. Hence, Eq.(D.153) must be fulfilled.

$$\sum_{\text{l}} \text{Amount}_{\text{l,j,year}} = \sum_{\text{group}} \text{TotalAmountCA}_{\text{j,year,group}} +$$
$$\sum_{\text{group}} \text{TotalAmountY}_{\text{j,year,group}} + \sum_{\text{group}} \text{TotalAmountCO}_{\text{j,year,group}} \forall j, year \tag{D.153}$$

It is necessary to differentiate between the part of the crop that is fed to animals ($\text{Amount}_{l,BarleyStraw,year}$, $\text{Amount}_{l,BarleyGrain,year}$, $\text{Amount}_{l,WheatGrain,year}$, and $\text{Amount}_{l,WheatStraw,year}$) and the part that is to be sold ($\text{sale}_{l,BarleyStraw,year}$, $\text{sale}_{l,BarleyGrain,year}$, $\text{sale}_{l,Wheatgrain,year}$, and $\text{sale}_{l,Wheatstraw,year}$). Eqs.(D.154) and (D.155) relate the 8 variables through the ratio of grain to straw in these two crops (0.53 for barley and 0.54 for wheat).

$$\text{Amount}_{\text{l,barleystraw,year}} + Sale_{\text{l,barleystraw,year}} =$$
$$0.53^*(\text{Amount}_{\text{l,barleygrain,year}} + \text{Sale}_{\text{l,barleygrain,year}}) \; \forall l, year \tag{D.154}$$

$$\text{Amount}_{\text{l,wheatstraw,year}} + Sale_{\text{l,wheatstraw,year}} =$$
$$0.54^*(\text{Amount}_{\text{l,wheatgrain,year}} + \text{Sale}_{\text{l,wheatgrain,year}}) \; \forall l, year \tag{D.155}$$

Since the main economic exploitation is the sale of meat, if an ingredient is chosen as feed, it cannot also be used for sale. For this purpose, a series of restrictions (Eqs.(D.156)-(D.161)) controlled by binary variables are introduced in the model.

$$Sale_{\mathrm{l,BarleyStraw,year}} - 10^4 \cdot \mathrm{bi1}_{\mathrm{l,year}} \leq 0;\ \forall l, year \tag{D.156}$$

$$Sale_{\mathrm{l,BarleyGrain,year}} - 10^4 \cdot \mathrm{bi2}_{\mathrm{l,year}} \leq 0;\ \forall l, year \tag{D.157}$$

$$Sale_{\mathrm{l,Wheatgrain,year}} - 10^4 \cdot \mathrm{bi3}_{\mathrm{l,year}} \leq 0;\ \forall l, year \tag{D.158}$$

$$Sale_{\mathrm{l,WheatStraw,year}} - 10^4 \cdot \mathrm{bi4}_{\mathrm{l,year}} \leq 0;\ \forall l, year \tag{D.159}$$

$$bi1_{l,year} + \mathrm{bi2}_{\mathrm{l,year}} = 1\ ;\ \forall l, year \tag{D.160}$$

$$bi3_{l,year} + \mathrm{bi4}_{\mathrm{l,year}} = 1\ ;\ \forall l, year \tag{D.161}$$

In addition, demand quantities can be covered by irrigated or rainfed crops (Eq.(D.162)).

$$\mathrm{Amount}_{\mathrm{l,j,year}}{=}\mathrm{AmountR}_{\mathrm{l,j,year}} + \mathrm{AmountS}_{\mathrm{l,j,year}}\ \forall l, j, year \tag{D.162}$$

It is possible to determine the area of crops needed to satisfy feed demand using the production values for each region (Tables D.12-D.13) and Eqs.(D.163) and (D.164).

$$\mathrm{AmountS}_{\mathrm{l,j,year}}{=}\mathrm{AreaS}_{\mathrm{l,j,year}} \cdot \mathrm{Pr}\,oductionS_{l,j,year}\ \forall l, j, year \tag{D.163}$$

$$\mathrm{AmountR}_{\mathrm{l,j,year}}{=}\mathrm{AreaR}_{\mathrm{l,j,year}} \cdot \mathrm{Production}_{\mathrm{l,j,year}}\ \forall l, j, year \tag{D.164}$$

Where $\mathrm{AreaS}_{l,j,year}$ and $\mathrm{AreaR}_{l,j,year}$ are the areas occupied by rainfed and irrigated 'j' crops, respectively, in 'l' region in 'year'. $\mathrm{ProductionS}_{l,j,year}$ and $\mathrm{ProducctionR}_{l,j,year}$ are the yields of crop 'j' in region 'l'. To determine which location is to be selected (since only one location is selected and it is the same for both irrigated and rainfed crops), Eq.(D.165), Eq.(D.166) and (D.167) are added to the model. As only one location is selected, Eq.(D.168) is included as well.

$$\mathrm{AmountS}_{\mathrm{l,j,year}} - \mathrm{selbi1}_{\mathrm{l}} \cdot 10^6 \leq 0\ \forall l, j, year \tag{D.165}$$

$$\mathrm{AmountR}_{\mathrm{l,j,year}} - \mathrm{selbi2}_{\mathrm{l}} \cdot 10^{6} \leq 0 \ \forall l, j, year \tag{D.166}$$

$$selbi1_{l} = selbi2_{l} \ \forall l \tag{D.167}$$

$$\sum_{l} selbi1_{l} = 1 \tag{D.168}$$

Only a part of the total available area is considered for the farm. For this purpose, Eq.(D.169) and Eq.(D.170) are introduced.

$$AreaS_{j,l,year} < fc \cdot AreaAvaS_{j,l} \ \forall l, j, year \tag{D.169}$$

$$AreaR_{j,l,year} < fc \cdot AreaAvaR_{j,l} \ \forall l, j, year \tag{D.170}$$

Where fc is the percentage used of the total available, while $\mathrm{AreaAvaS}_{j,l}$ and $\mathrm{AreaAvaR}_{j,l}$ is the total available crop area in region 'l' of ingredient 'j'. Finally, the amount of water consumed by both animals and irrigated crops must be less than available. A maximum consumption of 1% of the water available for irrigation and livestock in each county is set (Eq.(D.171)).

$$(\mathrm{CAA}j \cdot AreaR_{l,year}) + WaterF + WaterP < 0.01 \cdot WaterAvaR_{l} \ \forall l, year \tag{D.171}$$

Where $\mathrm{WaterAvaRl}_{l}$ is the water available at each location. WaterF and WaterP are the water consumed by the animals and the water consumed by the waste treatment process.

D.6 SOLUTION PROCEDURE

The income from the animals (Imt) is the sum of the income from the sale of meat of cows (In_{cows}), male yearling ($\mathrm{In}_{YearlingM}$) and female yearling ($\mathrm{In}_{YearlingF}$), which are estimated by Eqs.(D.172)-(D.174).

$$\mathrm{In}_{\mathrm{Cows}} = \sum_{group} (\mathrm{NA}_{\mathrm{Cows}})_{group} \cdot \mathrm{Pri}_{\mathrm{Cow}} \tag{D.172}$$

$$\mathrm{In}_{\mathrm{YearlingM}} = \sum_{group} (\mathrm{NA}_{\mathrm{YearlingM}})_{\mathrm{group}} \cdot \mathrm{Pri}_{\mathrm{YearlingM}} \tag{D.173}$$

$$\mathrm{In}_{\mathrm{YearlingF}} = \sum_{group} (\mathrm{NA}_{\mathrm{YearlingF}})_{group} \cdot \mathrm{Pri}_{\mathrm{YearlingF}} \tag{D.174}$$

The price of yearlings ($\mathrm{Pri}_{YearlingM}$ and $\mathrm{Pri}_{YearlingF}$) can be estimated using its final weight, meat yield (Huerta-Leidenz et al., 2013), and the official price of the meat from the literature, whereas the price of the cows (Pri_{Cow}) is fixed, 504€/cow. $\mathrm{Pri}_{yearlingM}$ is 516€/yearling and PriyearlingF is 685€/yearling (Lonja de Salamanca, 2021). $\mathrm{NA}_{cows_{group}}$, $\mathrm{NA}_{YearlingM_{group}}$, and $\mathrm{NA}_{YearlingF_{group}}$ are the number of cows, male yearling, and female yearling of each population group, respectively. The income obtained from the selling of barley and wheat (In_{crops}) is estimated by Eq.(D.175).

$$\mathrm{In}_{\mathrm{Crops}} = \mathrm{Sale}_{\mathrm{l,BarleyGrain,year}} \cdot \mathrm{Pri}_{\mathrm{Barley}} + \mathrm{Sale}_{\mathrm{l,BarleyStraw,year}} \cdot \mathrm{Pri}_{\mathrm{Barley.Straw}} + \mathrm{Sale}_{\mathrm{l,WheatGrain,year}} \cdot \mathrm{Pri}_{Wheat} + \mathrm{Sale}_{\mathrm{l,WheatStraw,year}} \cdot \mathrm{Pri}_{Wheat.Straw} \tag{D.175}$$

Where the price of barley grain (Pri_{Barley}), barley straw ($\mathrm{Pri}_{BarleyStraw}$), wheat grain ($\mathrm{Pri}_{Wheat}$) and wheat straw ($\mathrm{Pri}_{WheatStraw}$) are shown in Table D.5. The income of biogas (In_{bio}) is calculated, using the amount of biogas (Amt_{biogas}), the yield to produce power(yd), the heat of combustion (Hc), and the sale price of power (Pri_{power}). Therefore, the Eq.(D.176) is added to the model. The value of these parameters is 0.4 (IDAE, 2020), 14 kWh/kgbiogas (IDAE, 2020) and 200€/MWh (Llorens, 2018), respectively.

$$\mathrm{In}_{\mathrm{bio}} = \mathrm{Amt}_{biogas} \cdot \mathrm{yd} \cdot \mathrm{Pri}_{\mathrm{power}} \cdot HC \tag{D.176}$$

Regarding costs, Cst_{Crops} is the cost of production of the crop fed to calves (Cst_{Calves}), yearlings ($\mathrm{Cst}_{Yearling}$), cows (Cst_{Cow}) and bulls (Cst_{Bulls}) (Eq. (D.177)).

$$\mathrm{Cst}_{\mathrm{Crops}} = \mathrm{Cst}_{\mathrm{Calves}} + \mathrm{Cst}_{\mathrm{Yearling}} + \mathrm{Cst}_{\mathrm{Cow}} + \mathrm{Cst}_{\mathrm{Bull}} \tag{D.177}$$

The growing cost of calves (Cst_{Calves}), yearlings ($\mathrm{Cst}_{Yearling}$), cows(Cst_{Cow}), and bulls(Cst_{Bull}) are calculated by Eqs.(D.178)-(D.181).

$$\mathrm{Cst}_{\mathrm{Calves}} = \sum_{group} \sum_{\mathrm{t=0}}^{6} \mathrm{DMI}_{\mathrm{t,group}} \cdot \mathrm{CstM}_{\mathrm{t,group}} \cdot \mathrm{NA}_{\mathrm{calves}_{group}} \tag{D.178}$$

$$\mathrm{Cst}_{\mathrm{Yearling}} = \sum_{group} \sum_{\mathrm{t=7}}^{20} \mathrm{DMI}_{\mathrm{t,group}} \cdot \mathrm{CstM}_{\mathrm{t,group}} \cdot \mathrm{NA}_{\mathrm{yearling}_{group}} \tag{D.179}$$

$$\mathrm{Cst}_{\mathrm{Cow}} = \sum_{group} \sum_{\mathrm{t=21}}^{72} \mathrm{DMI}_{\mathrm{t,group}} \cdot \mathrm{CstM}_{\mathrm{t,group}} \cdot \mathrm{NA}_{\mathrm{cows}_{group}} \tag{D.180}$$

$$\mathrm{Cst_{Bulls}} = \sum_{group}\sum_{t=21}^{72} \mathrm{DMI_{t,group}} \cdot \mathrm{CstM_{t,group}} \cdot \mathrm{NA}_{\mathrm{Bulls}_{group}} \quad (D.181)$$

Where $\mathrm{CstM}_{t,group}$ is the crop production cost of feed in the period 't' for the population group 'group' and $\mathrm{DMI}_{t,group}(Kg/TU)$ is the amount of dry matter intake in a time period 't'. $\mathrm{NA}_{calves_{group}}$, $\mathrm{NA}_{yearling_{group}}$, $\mathrm{NA}_{bulls_{group}}$ are the number of calves, yearlings, and bulls in each group, respectively. The crop production cost of each ingredient (Cst_j) only includes the tillage, sowing, and harvesting (see Table D.5). ($\mathrm{CstM}_{t,group}$) is calculated by applying the composition of feed ($x_{t,j,group}$) and Cst_j(Eq.(D.182)).

$$\mathrm{Cs}\,tM_{t,group} = \sum_j Cst_j \cdot x_{t,j,group} \forall t, group \quad (D.182)$$

The rest of the costs (i.e, renting of field (Cst_{Field}), fertilizers ($\mathrm{Cst}_{Fertilizer}$), storage ($\mathrm{Cst}_{Storage}$), and labor ($\mathrm{Cst}_{labor}$)) are calculated by Eqs.(D.183)-(D.186).

$$\mathrm{Cst_{Field}} = \sum_l \sum_j \sum_{year} \mathrm{PriS}_{\mathrm{Rent}_l} \cdot \mathrm{AreaS}_{j,l,year} + \mathrm{PriR}_{\mathrm{Rent}_l} \cdot \mathrm{AreaR}_{j,l,year} \quad (D.183)$$

$$\mathrm{Cst_{Fertilizer}} = \mathrm{Amt_N} \cdot \mathrm{Pri_N} + \mathrm{Amt_P} \cdot \mathrm{Pri_P} + \mathrm{Amt_K} \cdot \mathrm{Pri_K} \quad (D.184)$$

$$\mathrm{Cst_{Storage}} = \mathrm{Pri_{storage}} \cdot \left(\sum_{\mathrm{t}} \sum_{group} \mathrm{DMI_{t,group}}\right) \cdot \frac{\mathrm{LC_{farm}}}{\mathrm{LC_{silo}}} \quad (D.185)$$

$$\mathrm{Cst_{Labor}} = \sum_{j,l,year} \mathrm{Pri_{MP}} \cdot (\mathrm{AreaS_{j,l,year}} + \mathrm{AreaR_{j,l,year}}) \quad (D.186)$$

Regarding Cst_{field}, Pri_{Srent_l} and Pri_{Rrent_l} are the rental price of rainfed and irrigated field in each location 'l', respectively (see Table D.9). $\mathrm{AreaS}_{j,l,year}$ and $\mathrm{AreaR}_{j,l,year}$ are the rainfed and irrigated cultivated area of crop 'j' in the location 'l' the year 'year'. The prices of the mineral fertilizers are 334.2€/t (ammonium nitrate (Pri_N)), 202€/t (perphosphate (Prin_P)), and 353 €/t (potassium sulfate (Prin_K)) (Ministerio de agricultura pesca y alimentación, 2020). The price of storing ($\mathrm{Pri}_{storage}$) the crops is 26€/t (Taifouris & Martin, 2021). LC_{silo} is the life cycle of the silo (25 years) while

LC_{farm} is the life cycle of the farm (20 years). The cost of labor is calculated using the price of labor per unit of area (Pri_{MP}), whose value is 50€/ha (Ministerio de Agricultura Pesca y Alimentación, 2017). Auxiliary costs ($CstAux$) are constituted by the cost of irrigation water ($Cst_{waterAgri}$), the cost of feed water ($Cst_{waterLiv}$) and the cost of feed supplements (Cst_{supl}). These costs are calculated by Eqs.(D.187)-(D.189).

$$\mathrm{Cst_{waterAgri}} = \mathrm{CstU_{waterAgri_l}} \cdot (\mathrm{CAA}_j \cdot AreaR_{l,j,year}) \tag{D.187}$$

Where $CostUWater_l$ is the unit price (€/m^3) of irrigation water and depends on the selected region. CAA_j is the annual water consumption of the crop 'j' and $AreaR_{l,j,year}$,year is the cultivation area of the crop 'j' in the region 'l' en the year 'year'.

$$\begin{aligned}\mathrm{Cst_{waterLiv}} = {} & (\mathrm{Wa_{Calves}} \cdot \mathrm{NA_{Calves_{group}}} \cdot \mathrm{lt_{Calves}} + \mathrm{Wa_{Yearling}} \cdot \mathrm{NA_{Yearling_{group}}} \\ & \cdot \mathrm{lt_{Yearling}} + \mathrm{Wa_{cows}} \cdot \mathrm{NA_{cows_{group}}} \cdot \mathrm{lt_{cows}}) \cdot CstU_{waterliv_l}\end{aligned} \tag{D.188}$$

Where Wa_{Calves}, $Wa_{yearling}$, and Wa_{Cows} are the consumption of water per day of calves, yearling and cows and their values are 3.5,25,70 liters (Lanuza, 2006; Duarte, 2011) , respectively. lt_{Calves}, $lt_{yearling}$ and It_{Cows} are the lifetime of those animals that is 168 days, 360 days and 1200 days. $Cst_{Uwaterlivl}$ is the unit cost of livestock water and depends on location.

$$\mathrm{Cst_{Supl}} = \mathrm{Amt_{supP}} \cdot \mathrm{Price_{supP}} + \mathrm{Amt_{supCa}} \cdot \mathrm{Price_{supCa}} \tag{D.189}$$

The price of mono-sodium phosphate (Pri_{supP}) is € 1.2 / kg (Echemi, 2021) and the price of calcium carbonate (Pri_{supCa}) is € 0.065 / kg (El confidencial químico, 2016) . To estimate the total cost of waste treatment and nutrient recovery, Eq.(D.190) is used.

$$Cst_{Wtre} = \sum_{group} \sum_{t} \mathrm{FEDM}_{t,group}(\mathrm{g/day}) \cdot CstU_{Wtre} \tag{D.190}$$

Where $CstU_{Wtre}$ is the unit cost of waste treatment and nitrogen recovery, which in the case of the transmembrane chemisorption is 0.025USD/kg-waste (Edgar, 2022). In addition, a new constraint must be added in the optimization framework to limit the use of the supplement of phosphorus Eq.(D.191).

$$\mathrm{Amt_{Supl_{t,grop}}} \leq \mathrm{Pneed_{t,group}} \tag{D.191}$$

D.7 MUTI-OBJECTIVE RESULTS

Table D.7 shows the completed results from techno-economic analysis of Section 3.2 of the manuscript.

Table D.7: .-Techno-economic analysis of the economic, multi-objective and eco-friendly scenario(Nd: needed, Rd:required)

Economic Scenario						
Income and cost	Amount(M€)	Crop	Amount(t)	Area(Ha)	Index	
Meat income	7.061	Corn Forage	675	19.27	GWP(tCO2)	15141
Crop Income	12.836	Alfalfa	29800	694.64	Eui(kgPO4-)	4330
Biogas Income	0.001	Vetch	289	13.20	Green Water Footprint(dam3)·0.1	5053
Field Cost	1.508	Barley Straw	41481	33414.97	Blue Water Footprint (dam3)·0.1	0
Fertilizer Cost	5.050	Barley Grain	2896		WF(dam3)·0.1	6401
Storage Cost	0.374	Barley Forage	0	0.00	N Nd(t)	4271
Labor Cost	0.584	Oat	0	0.00	P Nd(t)	3244
Crop Cost	4.624	Wheat Straw	4165	2689.54	K Nd(t)	4667
Wate Treatment Cost	2.434	Wheat Grain	4646		N Rd(t)	932
Aux Cost	0.359	Rye	8706	1582.96	P Rd(t)	2
Profit	4.965	Total	91983	38414.58	K Rd(t)	2486
Multi-objective Scenerio						
Income and cost	Amount(M€)	Crop	Amount(t)	Area(Ha)	Index	
Meat income	7.061	Corn Forage	675	19.27	GWP(tCO2)	12241
Crop Income	11.328	Alfalfa	35130	818.88	Eui(kgPO4-)	3601
Biogas Income	0.000	Vetch	288	13.15	Green Water Footprint(dam3)·0.1	4971
Field Cost	1.308	Barley Straw	37321	30109.82	Blue Water Footprint (dam3)·0.1	0
Fertilizer Cost	3.972	Barley Grain	4105		WF(dam3)·0.1	6343
Storage Cost	0.377	Barley Forage	781	29.70	N Nd(t)	3743
Labor Cost	0.507	Oat	744	135.33	P Nd(t)	2824
Crop Cost	4.652	Wheat Straw	3824	2112.40	K Nd(t)	4160
Wate Treatment Cost	2.474	Wheat Grain	2819		N Rd(t)	979
Aux Cost	0.354	Rye	8590	1561.81	P Rd(t)	3
Profit	4.745	Total	93602	34800.35	K Rd(t)	2580
Eco-friendly Scenario						
Income and cost	Amount(M€)	Crop	Amount(t)	Area(Ha)	Index	
Meat income	7.061	Corn Forage	548	15.67	GWP(tCO2)	10389
Crop Income	8.798	Alfalfa	32551	758.77	Eui(kgPO4-)	2706
Biogas Income	0.001	Vetch	258	11.78	Green Water Footprint(dam3)·0.1	5020
Field Cost	1.170	Barley Straw	34728	28048.72	Blue Water Footprint (dam3)·0.1	0
Fertilizer Cost	3.300	Barley Grain	11455		WF(dam3)·0.1	6388
Storage Cost	0.378	Barley Forage	1226	46.61	N Nd(t)	3486
Labor Cost	0.454	Oat	8796	1599.20	P Nd(t)	1685
Crop Cost	4.955	Wheat Straw	3434	2014.31	K Nd(t)	3868
Wate Treatment Cost	2.480	Wheat Grain	3007		N Rd(t)	975
Aux Cost	0.352	Rye	728	132.36	P Rd(t)	5
Profit	2.771	Total	96182	32627.41	K Rd(t)	2516

D.8 PROPERTIES OF AGRICULTURAL DISTRICTS

A total of 345 regions agricultural districts throughout Spain are considered. The price and availability of water, land rental price, available rainfed and irrigated area, as well as production yield of both types of crops for each region are shown in Table D.8-D.13. To estimate the availability of crops by agricultural district from the information on the availability of crops by provinces, the following approximation is used. Crop information is available for each of the agricultural distrits, but it is outdated (Gónzalez, 2013). By analyzing the updated information on crops by province(Ministerio de Agricultura pesca y alimentación, 2019b), and assuming a homogeneous growth of crops in each of the regions, it is possible to estimate the rainfed and irrigated crops in each region. For example, if in a province, 40% of rainfed crops are found in a specific region, this percentage is maintained in the following years. Thus, if the crops in that province increase in recent years, 40% of the total rainfed crops will continue to be allocated to that region. In other words, the distribution of crops by region, in the same province, remains the same, even though the amount of these crops increases or decreases over the years. This approximation has been chosen considering that crop yields depend on the climate and the nature and quality of the soils, and it has been assumed that these factors have not changed considerably from 2014 to the present.

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
Aguilar	1	8.00E-03	4.70E-02
AlbadeTormes	2	8.00E-03	4.70E-02
Alburquerque	3	4.08E-02	1.40E-02
Alcarria	4	4.08E-02	1.40E-02
AlcarriaAlta	5	1.10E-01	2.90E-02
AlcarriaBaja	6	1.10E-01	2.90E-02
Alhama	7	3.65E-01	6.40E-02
Aliste	8	8.00E-03	4.70E-02
Almansa	9	1.66E-01	2.90E-02
Almazan	10	8.00E-03	4.70E-02
Almendralejo	11	4.08E-02	1.40E-02
AltoAlmanzora	12	3.65E-01	6.40E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
AltoAmpurdan	13	5.11E-02	3.50E-02
AltoAndarax	14	3.65E-01	6.40E-02
AltoMaestrazgo	15	2.00E-01	8.00E-02
AltoTuria	16	2.00E-01	8.00E-02
AltoUrgel	17	5.11E-02	3.50E-02
AndevaloOccidental	18	1.90E-01	9.88E-02
AndevaloOriental	19	1.90E-01	9.88E-02
Anoia	20	5.11E-02	3.50E-02
Antequera	21	3.65E-01	6.40E-02
Aranga	22	5.00E-02	6.00E-02
ArcosdeJalon	23	8.00E-03	4.70E-02
AreaMetro-politana	24	1.10E-01	2.90E-02
Arevalo-Madrigal	25	1.10E-01	2.90E-02
Arlanza	26	8.00E-03	4.70E-02
Arlanzon	27	8.00E-03	4.70E-02
Arzua	28	5.00E-02	6.00E-02
Ason	29	1.49E-01	1.00E+03
Astorga	30	8.00E-03	4.70E-02
Avila	31	1.10E-01	2.90E-02
Azuaga	32	4.08E-02	1.40E-02
Badajoz	33	4.08E-02	1.40E-02
Bages	34	5.11E-02	3.50E-02
BajoAlmanzora	35	3.65E-01	6.40E-02
BajoAmpurdan	36	5.11E-02	3.50E-02
BajoAragon	37	2.00E-01	8.00E-02
BajoCinca	38	2.08E-01	2.00E-02
BajoEbro	39	5.11E-02	3.50E-02
BajoLlobregat	40	5.11E-02	3.50E-02
BajoMaestrazgo	41	2.00E-01	8.00E-02
BajoPenedes	42	5.11E-02	3.50E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
BarcodeAvila-Piedrahita	43	1.10E-01	2.90E-02
Baza	44	3.65E-01	6.40E-02
BelmontedeMiranda	45	1.49E-01	1.00E+03
BenaventeylosValles	46	8.00E-03	4.70E-02
Bergada	47	5.11E-02	3.50E-02
Bierzo	48	8.00E-03	4.70E-02
Boedo-Ojeda	49	8.00E-03	4.70E-02
Boimorto	50	5.00E-02	6.00E-02
Borja	51	2.08E-01	2.00E-02
Brozas	52	1.10E-01	2.90E-01
Bureba-Ebro	53	8.00E-03	4.70E-02
BurgodeOsma	54	8.00E-03	4.70E-02
Caceres	55	1.10E-01	2.90E-01
Calatayud	56	2.08E-01	2.00E-02
Campina	57	1.10E-01	2.90E-02
Campina	58	1.10E-01	2.90E-02
CampinaAlta	59	1.12E-01	6.40E-02
CampinaBaja	60	1.12E-01	6.40E-02
CampinadeCadiz	61	1.90E-01	3.35E-02
CampinaNorte	62	1.12E-01	6.40E-02
CampinaSur	63	1.12E-01	6.40E-02
CampoDalias	64	3.65E-01	6.40E-02
CampodeCalatrava	65	4.08E-02	1.40E-02
CampodeCartagena	66	1.66E-01	2.90E-02
CampodeGibraltar	67	1.90E-01	4.71E-02
CampodeMontiel	68	4.08E-02	1.40E-02
CampodeTarragona	69	5.11E-02	3.50E-02
CampoNijar	70	3.65E-01	6.40E-02
CampoTabernas	71	3.65E-01	6.40E-02
Campos	72	8.00E-03	4.70E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
CamposdeGomara	73	8.00E-03	4.70E-02
CamposdeLiria	74	2.00E-01	8.00E-02
Campos-Pan	75	8.00E-03	4.70E-02
CangasdeNarcea	76	1.49E-01	1.00E+03
CangasdeOnis	77	1.49E-01	1.00E+03
Cantabrica	78	2.08E-01	2.00E-02
Capela	79	5.00E-02	6.00E-02
Caspe	80	2.08E-01	2.00E-02
Castuera	81	4.08E-02	1.40E-02
Central	82	1.30E-02	7.33E-03
Central	83	2.00E-01	8.00E-02
Centro	84	8.00E-03	4.70E-02
Centro	85	1.66E-01	2.90E-02
Centro	86	1.66E-01	2.90E-02
Cerceda	87	5.00E-02	6.00E-02
Cerdana	88	5.11E-02	3.50E-02
Cervera	89	8.00E-03	4.70E-02
CiudadRodrigo	90	8.00E-03	4.70E-02
Conca	91	5.11E-02	3.50E-02
ConcadeBarbera	92	5.11E-02	3.50E-02
CondadoCampina	93	1.90E-01	9.88E-02
CondadoLitoral	94	1.90E-01	9.88E-02
Coria	95	1.10E-01	2.90E-01
Costa	96	1.30E-02	7.33E-03
Costa	97	1.90E-01	9.88E-02
CostaNoroeste	98	1.90E-01	4.71E-02
Costera	99	1.49E-01	1.00E+03
Cuellar	100	8.00E-03	4.70E-02
CuencadelJiloca	101	2.00E-01	8.00E-02
CuencaPamplona	102	2.08E-01	2.00E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
Curtis	103	5.00E-02	6.00E-02
Daroca	104	2.08E-01	2.00E-02
DeEstepa	105	1.12E-01	6.40E-02
DelaJanda	106	1.90E-01	3.35E-02
DelaVega	107	3.65E-01	6.40E-02
Demanda	108	8.00E-03	4.70E-02
DonBenito	109	4.08E-02	1.40E-02
DueroBajo	110	8.00E-03	4.70E-02
EjeadelosCaballeros	111	2.08E-01	2.00E-02
ElAljarafe	112	1.12E-01	6.40E-02
ElBarcodeValdeorras	113	1.30E-02	7.33E-03
ElCerrato	114	8.00E-03	4.70E-02
ElCondado	115	1.12E-01	6.40E-02
ElParamo	116	8.00E-03	4.70E-02
EnguerayLaCanal	117	2.00E-01	8.00E-02
Esla-Campos	118	8.00E-03	4.70E-02
EstribacionesGorbea	119	2.08E-01	2.00E-02
Frades	120	5.00E-02	6.00E-02
FuentedeSanEsteban	121	8.00E-03	4.70E-02
Fuerteventura	122	8.28E-02	1.70E-01
Gandia	123	2.00E-01	8.00E-02
Garrigas	124	5.11E-02	3.50E-02
Garrotxa	125	5.11E-02	3.50E-02
Gijon	126	1.49E-01	1.00E+03
Girones	127	5.11E-02	3.50E-02
Grado	128	1.49E-01	1.00E+03
GranCanaria	129	8.28E-02	1.70E-01
Gredos	130	1.10E-01	2.90E-02
Guadalorce	131	3.65E-01	6.40E-02
Guadarrama	132	1.10E-01	2.90E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
Guadix	133	3.65E-01	6.40E-02
Guardo	134	8.00E-03	4.70E-02
Guipuzcoa	135	3.44E-01	1.00E+03
Hellin	136	1.66E-01	2.90E-02
HerreraDuque	137	4.08E-02	1.40E-02
Hervas	138	1.10E-01	2.90E-01
HoyadeBunol	139	2.00E-01	8.00E-02
HoyadeHuesca	140	2.08E-01	2.00E-02
HoyadeTeruel	141	2.00E-01	8.00E-02
HuertadeValencia	142	2.00E-01	8.00E-02
Huescar	143	3.65E-01	6.40E-02
Ibiza	144	2.13E-01	1.80E-01
Interior	145	1.30E-02	7.33E-03
Irixoa	146	5.00E-02	6.00E-02
IsladeElHierro	147	7.00E-01	7.00E-01
IsladeLaGomera	148	7.00E-01	7.00E-01
IsladeLaPalma	149	7.00E-01	7.00E-01
Iznalloz	150	3.65E-01	6.40E-02
Jacetania	151	2.08E-01	2.00E-02
JaraizdelaVera	152	1.10E-01	2.90E-01
JerezdelosCaballeros	153	4.08E-02	1.40E-02
LaAlmuniadeDonaGodina	154	2.08E-01	2.00E-02
LaBaneza	155	8.00E-03	4.70E-02
LaCabrera	156	8.00E-03	4.70E-02
LaCampina	157	1.12E-01	6.40E-02
LaCosta	158	3.65E-01	6.40E-02
LaCosteradeJativa	159	2.00E-01	8.00E-02
LaJara	160	1.10E-01	2.90E-02
LaLitera	161	2.08E-01	2.00E-02
LaLoma	162	1.12E-01	6.40E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
LaMancha	163	1.10E-01	2.90E-02
LaMontanadeLuna	164	8.00E-03	4.70E-02
LaMontanadeRiano	165	8.00E-03	4.70E-02
LaPlana	166	2.00E-01	8.00E-02
LaRibera	167	8.00E-03	4.70E-02
LaSelva	168	5.11E-02	3.50E-02
LaSierra	169	8.00E-03	4.70E-02
LaSierra	170	8.00E-03	6.40E-02
LaSierraNorte	171	1.12E-01	6.40E-02
LaSierraSur	172	1.12E-01	6.40E-02
LaVega	173	1.12E-01	6.40E-02
Lanzarote	174	8.28E-02	1.70E-01
LasAlpujarras	175	3.65E-01	6.40E-02
LasColonias	176	1.12E-01	6.40E-02
LasMarismas	177	1.12E-01	6.40E-02
Ledesma	178	8.00E-03	4.70E-02
Liebana	179	1.49E-01	1.00E+03
Litoral	180	1.30E-02	7.33E-03
LitoralNorte	181	2.00E-01	8.00E-02
LlanadaAlavesa	182	2.08E-01	2.00E-02
Llanes	183	1.49E-01	1.00E+03
LlanosCentrales	184	2.00E-01	8.00E-02
Llerena	185	4.08E-02	1.40E-02
Logrosan	186	1.10E-01	2.90E-01
LosVelez	187	3.65E-01	6.40E-02
LozoyaSomosierra	188	1.10E-01	2.90E-02
Luarca	189	1.49E-01	1.00E+03
Maestrazgo	190	2.00E-01	8.00E-02
Magina	191	1.12E-01	6.40E-02
Mallorca	192	2.13E-01	1.80E-01

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
Man-chuela	193	1.66E-01	2.90E-02
Mancha	194	1.66E-01	2.90E-02
Mancha	195	4.08E-02	1.40E-02
ManchaAlta	196	4.08E-02	1.40E-02
ManchaBaja	197	4.08E-02	1.40E-02
Manchuela	198	4.08E-02	1.40E-02
Maresme	199	5.11E-02	3.50E-02
Marquesado	200	2.00E-01	8.00E-02
Melide	201	5.00E-02	6.00E-02
Menorca	202	2.13E-01	1.80E-01
Merida	203	4.08E-02	1.40E-02
Meridional	204	2.00E-01	8.00E-02
Merindades	205	8.00E-03	4.70E-02
Mesia	206	5.00E-02	6.00E-02
Mieres	207	1.49E-01	1.00E+03
Mino	208	1.30E-02	7.33E-03
MolinadeAragon	209	1.10E-01	2.90E-02
Monegros	210	2.08E-01	2.00E-02
Monfero	211	5.00E-02	6.00E-02
Montana	212	1.30E-02	7.33E-03
Montana	213	1.30E-02	7.33E-03
Montana	214	2.00E-01	8.00E-02
MontanaAlavesa	215	2.08E-01	2.00E-02
MontedelosYebenes	216	1.10E-01	2.90E-02
Montefrio	217	3.65E-01	6.40E-02
MontesdeNavahermosa	218	1.10E-01	2.90E-02
MontesNorte	219	4.08E-02	1.40E-02
MontesSur	220	4.08E-02	1.40E-02
Moyanes	221	5.11E-02	3.50E-02
NavalmoraldelaMata	222	1.10E-01	2.90E-01

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
NavarraMedia	223	2.08E-01	2.00E-02
Noguera	224	5.11E-02	3.50E-02
NordOccidental	225	2.08E-01	2.00E-02
Nordeste	226	1.66E-01	2.90E-02
Noroeste	227	1.66E-01	2.90E-02
NortedeTenerife	228	7.00E-01	7.00E-01
Olivenza	229	4.08E-02	1.40E-02
Ordes	230	5.00E-02	6.00E-02
Oroso	231	5.00E-02	6.00E-02
Osona	232	5.11E-02	3.50E-02
Ourense	233	1.30E-02	7.33E-03
Oviedo	234	1.49E-01	1.00E+03
Palancia	235	2.00E-01	8.00E-02
Pallars-Ribagorza	236	5.11E-02	3.50E-02
Paramos	237	8.00E-03	4.70E-02
Pas-Iguna	238	1.49E-01	1.00E+03
Pastos	239	4.08E-02	1.40E-02
Pedroches	240	1.12E-01	6.40E-02
Penedes	241	5.11E-02	3.50E-02
Penibetica	242	1.12E-01	6.40E-02
Penagolosa	243	2.00E-01	8.00E-02
PenarandadeBraca-monte	244	8.00E-03	4.70E-02
Pinares	245	8.00E-03	4.70E-02
PinoO	246	5.00E-02	6.00E-02
Pirineos	247	2.08E-01	2.00E-02
Pisuerga	248	8.00E-03	4.70E-02
Plasencia	249	1.10E-01	2.90E-01
PontesdeG	250	5.00E-02	6.00E-02
Priorato-Prades	251	5.11E-02	3.50E-02
PueblaAlcocer	252	4.08E-02	1.40E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
Reinosa	253	1.49E-01	1.00E+03
Requena-Utiel	254	2.00E-01	8.00E-02
Ribagorza	255	2.08E-01	2.00E-02
RiberaAltaAragon	256	2.08E-01	2.00E-02
RiberaBaja	257	2.08E-01	2.00E-02
RiberadeEbro	258	5.11E-02	3.50E-02
RiberasdelJucar	259	2.00E-01	8.00E-02
RincondeAdemuz	260	2.00E-01	8.00E-02
RioNacimiento	261	3.65E-01	6.40E-02
RioSegura	262	1.66E-01	2.90E-02
RiojaAlavesa	263	2.08E-01	2.00E-02
RiojaAlta	264	2.08E-01	2.00E-02
RiojaBaja	265	2.08E-01	2.00E-02
RiojaMedia	266	2.08E-01	2.00E-02
Ripolles	267	5.11E-02	3.50E-02
Sagra-Toledo	268	1.10E-01	2.90E-02
Sagunto	269	2.00E-01	8.00E-02
Sahagun	270	8.00E-03	4.70E-02
Salamanca	271	8.00E-03	4.70E-02
Saldana-Valdavia	272	8.00E-03	4.70E-02
Sanabria	273	8.00E-03	4.70E-02
Santiso	274	5.00E-02	6.00E-02
Sayago	275	8.00E-03	4.70E-02
Segarra	276	5.11E-02	3.50E-02
Segarra	277	5.11E-02	3.50E-02
Segovia	278	8.00E-03	4.70E-02
Segria	279	5.11E-02	3.50E-02
Sepulveda	280	8.00E-03	4.70E-02
SerraniaAlta	281	4.08E-02	1.40E-02
SerraniaBaja	282	4.08E-02	1.40E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
SerraniadeAlbarracin	283	2.00E-01	8.00E-02
SerraniadeMontalban	284	2.00E-01	8.00E-02
SerraniadeRonda	285	3.65E-01	6.40E-02
SerraniaMedia	286	4.08E-02	1.40E-02
Sierra	287	1.10E-01	2.90E-02
Sierra	288	1.90E-01	9.88E-02
SierraAlcaraz	289	1.66E-01	2.90E-02
SierradeCadiz	290	1.90E-01	4.71E-02
SierradeCazorla	291	1.12E-01	6.40E-02
SierradeSegura	292	1.12E-01	6.40E-02
SierraMorena	293	1.12E-01	6.40E-02
SierraRiojaAlta	294	2.08E-01	2.00E-02
SierraRiojaBaja	295	2.08E-01	2.00E-02
SierraRiojaMedia	296	2.08E-01	2.00E-02
SierraSegura	297	1.66E-01	2.90E-02
SierraSur	298	1.12E-01	6.40E-02
Sobrado	299	5.00E-02	6.00E-02
Sobrarbe	300	2.08E-01	2.00E-02
Solsones	301	5.11E-02	3.50E-02
Somontano	302	2.08E-01	2.00E-02
Somozas	303	5.00E-02	6.00E-02
Soria	304	8.00E-03	4.70E-02
Sur	305	1.30E-02	7.33E-03
Sur	306	8.00E-03	4.70E-02
SurdeTenerife	307	7.00E-01	7.00E-01
SurOcci-dental	308	1.10E-01	2.90E-02
Sureste	309	8.00E-03	4.70E-02
SuroesteyValleGuadalentin	310	1.66E-01	2.90E-02
Talavera	311	1.10E-01	2.90E-02
TerraAlta	312	5.11E-02	3.50E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
TerraCha	313	1.30E-02	7.33E-03
TierradeCampos	314	8.00E-03	4.70E-02
TierraEstella	315	2.08E-01	2.00E-02
TierrasAltasyValledelTera	316	8.00E-03	4.70E-02
TierrasdeLeon	317	8.00E-03	4.70E-02
Toques	318	5.00E-02	6.00E-02
Tordoia	319	5.00E-02	6.00E-02
Torrijos	320	1.10E-01	2.90E-02
Touro	321	5.00E-02	6.00E-02
Trazo	322	5.00E-02	6.00E-02
Trujillo	323	1.10E-01	2.90E-01
Tudanca-Cabuerniga	324	1.49E-01	1.00E+03
Urgel	325	5.11E-02	3.50E-02
ValdoDubra	326	5.00E-02	6.00E-02
ValenciadeAlcantara	327	1.10E-01	2.90E-01
ValledeAran	328	5.11E-02	3.50E-02
ValledeAyora	329	2.00E-01	8.00E-02
ValledeLecrin	330	3.65E-01	6.40E-02
ValledelBajoAlberche	331	1.10E-01	2.90E-02
ValledelTietar	332	1.10E-01	2.90E-02
VallesAlaveses	333	2.08E-01	2.00E-02
VallesdeAlbaida	334	2.00E-01	8.00E-02
VallesOccidental	335	5.11E-02	3.50E-02
VallesOriental	336	5.11E-02	3.50E-02
Vegadeo	337	1.49E-01	1.00E+03
Vegas	338	1.10E-01	2.90E-02
Velez-Malaga	339	3.65E-01	6.40E-02
Verin	340	1.30E-02	7.33E-03
Vilasantar	341	5.00E-02	6.00E-02
Vinalopo	342	2.00E-01	8.00E-02

Table D.8: .-Price and availability of water (€/m^3) (Ministerio para la transición ecológica y reto demográfico, 2021)

Region	Code	Price (livestock)	Price (irrigiate crops)
Vitigudino	343	8.00E-03	4.70E-02
Vizcaya	344	3.44E-01	1.00E+03
Zaragoza	345	2.08E-01	2.00E-02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
Aguilar	1.29E+02	3.67E+02
AlbadeTormes	1.29E+02	3.67E+02
Alburquerque	7.90E+01	5.42E+02
Alcarria	7.40E+01	4.63E+02
AlcarriaAlta	7.40E+01	4.63E+02
AlcarriaBaja	7.40E+01	4.63E+02
Alhama	1.73E+02	6.68E+02
Aliste	1.29E+02	3.67E+02
Almansa	7.40E+01	4.63E+02
Almazan	1.29E+02	3.67E+02
Almendralejo	7.90E+01	5.42E+02
AltoAlmanzora	1.73E+02	6.68E+02
AltoAmpurdan	1.74E+02	4.26E+02
AltoAndarax	1.73E+02	6.68E+02
AltoMaestrazgo	5.70E+01	7.32E+02
AltoTuria	5.70E+01	7.32E+02
AltoUrgel	1.74E+02	4.26E+02
AndevaloOccidental	1.73E+02	6.68E+02
AndevaloOriental	1.73E+02	6.68E+02
Anoia	1.74E+02	4.26E+02
Antequera	1.73E+02	6.68E+02
Aranga	2.61E+02	2.66E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
ArcosdeJalon	1.29E+02	3.67E+02
AreaMetro-politana	4.90E+01	3.46E+02
Arevalo-Madrigal	1.29E+02	3.67E+02
Arlanza	1.29E+02	3.67E+02
Arlanzon	1.29E+02	3.67E+02
Arzua	2.61E+02	2.66E+02
Ason	2.08E+02	1.00E+05
Astorga	1.29E+02	3.67E+02
Avila	1.29E+02	3.67E+02
Azuaga	7.90E+01	5.42E+02
Badajoz	7.90E+01	5.42E+02
Bages	1.74E+02	4.26E+02
BajoAlmanzora	1.73E+02	6.68E+02
BajoAmpurdan	1.74E+02	4.26E+02
BajoAragon	8.00E+01	3.88E+02
BajoCinca	8.00E+01	3.88E+02
BajoEbro	1.74E+02	4.26E+02
BajoLlobregat	1.74E+02	4.26E+02
BajoMaestrazgo	5.70E+01	7.32E+02
BajoPenedes	1.74E+02	4.26E+02
BarcodeAvila-Piedrahita	1.29E+02	3.67E+02
Baza	1.73E+02	6.68E+02
BelmontedeMiranda	1.78E+02	1.00E+05
BenaventeylosValles	1.29E+02	3.67E+02
Bergada	1.74E+02	4.26E+02
Bierzo	1.29E+02	3.67E+02
Boedo-Ojeda	1.29E+02	3.67E+02
Boimorto	2.61E+02	2.66E+02
Borja	8.00E+01	3.88E+02
Brozas	7.90E+01	5.42E+02
Bureba-Ebro	1.29E+02	3.67E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
BurgodeOsma	1.29E+02	3.67E+02
Caceres	7.90E+01	5.42E+02
Calatayud	8.00E+01	3.88E+02
Campina	4.90E+01	3.46E+02
Campina	7.40E+01	4.63E+02
CampinaAlta	1.73E+02	6.68E+02
CampinaBaja	1.73E+02	6.68E+02
CampinadeCadiz	1.73E+02	6.68E+02
CampinaNorte	1.73E+02	6.68E+02
CampinaSur	1.73E+02	6.68E+02
CampoDalias	1.73E+02	6.68E+02
CampodeCalatrava	7.40E+01	4.63E+02
CampodeCartagena	1.13E+02	7.74E+02
CampodeGibraltar	1.73E+02	6.68E+02
CampodeMontiel	7.40E+01	4.63E+02
CampodeTarragona	1.74E+02	4.26E+02
CampoNijar	1.73E+02	6.68E+02
CampoTabernas	1.73E+02	6.68E+02
Campos	1.29E+02	3.67E+02
CamposdeGomara	1.29E+02	3.67E+02
CamposdeLiria	5.70E+01	7.32E+02
Campos-Pan	1.29E+02	3.67E+02
CangasdeNarcea	1.78E+02	1.00E+05
CangasdeOnis	1.78E+02	1.00E+05
Cantabrica	2.37E+02	1.00E+05
Capela	2.61E+02	2.66E+02
Caspe	8.00E+01	3.88E+02
Castuera	7.90E+01	5.42E+02
Central	2.61E+02	2.66E+02
Central	5.70E+01	7.32E+02
Centro	1.29E+02	3.67E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
Centro	7.40E+01	4.63E+02
Centro	1.13E+02	7.74E+02
Cerceda	2.61E+02	2.66E+02
Cerdana	1.74E+02	4.26E+02
Cervera	1.29E+02	3.67E+02
CiudadRodrigo	1.29E+02	3.67E+02
Conca	1.74E+02	4.26E+02
ConcadeBarbera	1.74E+02	4.26E+02
CondadoCampina	1.73E+02	6.68E+02
CondadoLitoral	1.73E+02	6.68E+02
Coria	7.90E+01	5.42E+02
Costa	2.61E+02	2.66E+02
Costa	1.73E+02	6.68E+02
CostaNoroeste	1.73E+02	6.68E+02
Costera	2.08E+02	1.00E+05
Cuellar	1.29E+02	3.67E+02
CuencadelJiloca	8.00E+01	3.88E+02
CuencaPamplona	1.95E+02	3.80E+02
Curtis	2.61E+02	2.66E+02
Daroca	8.00E+01	3.88E+02
DeEstepa	1.73E+02	6.68E+02
DelaJanda	1.73E+02	6.68E+02
DelaVega	1.73E+02	6.68E+02
Demanda	1.29E+02	3.67E+02
DonBenito	7.90E+01	5.42E+02
DueroBajo	1.29E+02	3.67E+02
EjeadelosCaballeros	8.00E+01	3.88E+02
ElAljarafe	1.73E+02	6.68E+02
ElBarcodeValdeorras	2.61E+02	2.66E+02
ElCerrato	1.29E+02	3.67E+02
ElCondado	1.73E+02	6.68E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
ElParamo	1.29E+02	3.67E+02
EnguerayLaCanal	5.70E+01	7.32E+02
Esla-Campos	1.29E+02	3.67E+02
EstribacionesGorbea	2.37E+02	1.00E+05
Frades	2.61E+02	2.66E+02
FuentedeSanEsteban	1.29E+02	3.67E+02
Fuerteventura	1.67E+03	3.82E+03
Gandia	5.70E+01	7.32E+02
Garrigas	1.74E+02	4.26E+02
Garrotxa	1.74E+02	4.26E+02
Gijon	1.78E+02	1.00E+05
Girones	1.74E+02	4.26E+02
Grado	1.78E+02	1.00E+05
GranCanaria	1.67E+03	3.82E+03
Gredos	1.29E+02	3.67E+02
Guadalorce	1.73E+02	6.68E+02
Guadarrama	4.90E+01	3.46E+02
Guadix	1.73E+02	6.68E+02
Guardo	1.29E+02	3.67E+02
Guipuzcoa	2.37E+02	1.00E+06
Hellin	7.40E+01	4.63E+02
HerreraDuque	7.90E+01	5.42E+02
Hervas	7.90E+01	5.42E+02
HoyadeBunol	5.70E+01	7.32E+02
HoyadeHuesca	8.00E+01	3.88E+02
HoyadeTeruel	8.00E+01	3.88E+02
HuertadeValencia	5.70E+01	7.32E+02
Huescar	1.73E+02	6.68E+02
Ibiza	9.50E+01	2.50E+02
Interior	2.61E+02	2.66E+02
Irixoa	2.61E+02	2.66E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
IsladeElHierro	1.67E+03	3.82E+03
IsladeLaGomera	1.67E+03	3.82E+03
IsladeLaPalma	1.67E+03	3.82E+03
Iznalloz	1.73E+02	6.68E+02
Jacetania	8.00E+01	3.88E+02
JaraizdelaVera	7.90E+01	5.42E+02
JerezdelosCaballeros	7.90E+01	5.42E+02
LaAlmuniadeDonaGodina	8.00E+01	3.88E+02
LaBaneza	1.29E+02	3.67E+02
LaCabrera	1.29E+02	3.67E+02
LaCampina	1.73E+02	6.68E+02
LaCosta	1.73E+02	6.68E+02
LaCosteradeJativa	5.70E+01	7.32E+02
LaJara	7.40E+01	4.63E+02
LaLitera	8.00E+01	3.88E+02
LaLoma	1.73E+02	6.68E+02
LaMancha	7.40E+01	4.63E+02
LaMontanadeLuna	1.29E+02	3.67E+02
LaMontanadeRiano	1.29E+02	3.67E+02
LaPlana	5.70E+01	7.32E+02
LaRibera	1.29E+02	3.67E+02
LaSelva	1.74E+02	4.26E+02
LaSierra	1.29E+02	3.67E+02
LaSierra	1.73E+02	3.67E+02
LaSierraNorte	1.73E+02	6.68E+02
LaSierraSur	1.73E+02	6.68E+02
LaVega	1.73E+02	6.68E+02
Lanzarote	1.67E+03	3.82E+03
LasAlpujarras	1.73E+02	6.68E+02
LasColonias	1.73E+02	6.68E+02
LasMarismas	1.73E+02	6.68E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
Ledesma	1.29E+02	3.67E+02
Liebana	2.08E+02	1.00E+05
Litoral	2.61E+02	2.66E+02
LitoralNorte	5.70E+01	7.32E+02
LlanadaAlavesa	2.37E+02	1.00E+05
Llanes	1.78E+02	1.00E+05
LlanosCentrales	5.70E+01	7.32E+02
Llerena	7.90E+01	5.42E+02
Logrosan	7.90E+01	5.42E+02
LosVelez	1.73E+02	6.68E+02
LozoyaSomosierra	4.90E+01	3.46E+02
Luarca	1.78E+02	1.00E+05
Maestrazgo	8.00E+01	3.88E+02
Magina	1.73E+02	6.68E+02
Mallorca	9.50E+01	2.50E+02
Man-chuela	7.40E+01	4.63E+02
Mancha	7.40E+01	4.63E+02
Mancha	7.40E+01	4.63E+02
ManchaAlta	7.40E+01	4.63E+02
ManchaBaja	7.40E+01	4.63E+02
Manchuela	7.40E+01	4.63E+02
Maresme	1.74E+02	4.26E+02
Marquesado	5.70E+01	7.32E+02
Melide	2.61E+02	2.66E+02
Menorca	9.50E+01	2.50E+02
Merida	7.90E+01	5.42E+02
Meridional	5.70E+01	7.32E+02
Merindades	1.29E+02	3.67E+02
Mesia	2.61E+02	2.66E+02
Mieres	1.78E+02	1.00E+05
Mino	2.61E+02	2.66E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
MolinadeAragon	7.40E+01	4.63E+02
Monegros	8.00E+01	3.88E+02
Monfero	2.61E+02	2.66E+02
Montana	2.61E+02	2.66E+02
Montana	2.61E+02	2.66E+02
Montana	5.70E+01	7.32E+02
MontanaAlavesa	2.37E+02	1.00E+05
MontedelosYebenes	7.40E+01	4.63E+02
Montefrio	1.73E+02	6.68E+02
MontesdeNavahermosa	7.40E+01	4.63E+02
MontesNorte	7.40E+01	4.63E+02
MontesSur	7.40E+01	4.63E+02
Moyanes	1.74E+02	4.26E+02
NavalmoraldelaMata	7.90E+01	5.42E+02
NavarraMedia	1.95E+02	3.80E+02
Noguera	1.74E+02	4.26E+02
NordOccidental	1.95E+02	3.80E+02
Nordeste	1.13E+02	7.74E+02
Noroeste	1.13E+02	7.74E+02
NortedeTenerife	1.67E+03	3.82E+03
Olivenza	7.90E+01	5.42E+02
Ordes	2.61E+02	2.66E+02
Oroso	2.61E+02	2.66E+02
Osona	1.74E+02	4.26E+02
Ourense	2.61E+02	2.66E+02
Oviedo	1.78E+02	1.00E+05
Palancia	5.70E+01	7.32E+02
Pallars-Ribagorza	1.74E+02	4.26E+02
Paramos	1.29E+02	3.67E+02
Pas-Iguna	2.08E+02	1.00E+05
Pastos	7.40E+01	4.63E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
Pedroches	1.73E+02	6.68E+02
Penedes	1.74E+02	4.26E+02
Penibetica	1.73E+02	6.68E+02
Penagolosa	5.70E+01	7.32E+02
PenarandadeBraca-monte	1.29E+02	3.67E+02
Pinares	1.29E+02	3.67E+02
PinoO	2.61E+02	2.66E+02
Pirineos	1.95E+02	3.80E+02
Pisuerga	1.29E+02	3.67E+02
Plasencia	7.90E+01	5.42E+02
PontesdeG	2.61E+02	2.66E+02
Priorato-Prades	1.74E+02	4.26E+02
PueblaAlcocer	7.90E+01	5.42E+02
Reinosa	2.08E+02	1.00E+05
Requena-Utiel	5.70E+01	7.32E+02
Ribagorza	8.00E+01	3.88E+02
RiberaAltaAragon	1.95E+02	3.80E+02
RiberaBaja	1.95E+02	3.80E+02
RiberadeEbro	1.74E+02	4.26E+02
RiberasdelJucar	5.70E+01	7.32E+02
RincondeAdemuz	5.70E+01	7.32E+02
RioNacimiento	1.73E+02	6.68E+02
RioSegura	1.13E+02	7.74E+02
RiojaAlavesa	2.37E+02	1.00E+05
RiojaAlta	1.47E+02	4.24E+02
RiojaBaja	1.47E+02	4.24E+02
RiojaMedia	1.47E+02	4.24E+02
Ripolles	1.74E+02	4.26E+02
Sagra-Toledo	7.40E+01	4.63E+02
Sagunto	5.70E+01	7.32E+02
Sahagun	1.29E+02	3.67E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
Salamanca	1.29E+02	3.67E+02
Saldana-Valdavia	1.29E+02	3.67E+02
Sanabria	1.29E+02	3.67E+02
Santiso	2.61E+02	2.66E+02
Sayago	1.29E+02	3.67E+02
Segarra	1.74E+02	4.26E+02
Segarra	1.74E+02	4.26E+02
Segovia	1.29E+02	3.67E+02
Segria	1.74E+02	4.26E+02
Sepulveda	1.29E+02	3.67E+02
SerraniaAlta	7.40E+01	4.63E+02
SerraniaBaja	7.40E+01	4.63E+02
SerraniadeAlbarracin	8.00E+01	3.88E+02
SerraniadeMontalban	8.00E+01	3.88E+02
SerraniadeRonda	1.73E+02	6.68E+02
SerraniaMedia	7.40E+01	4.63E+02
Sierra	7.40E+01	4.63E+02
Sierra	1.73E+02	6.68E+02
SierraAlcaraz	7.40E+01	4.63E+02
SierradeCadiz	1.73E+02	6.68E+02
SierradeCazorla	1.73E+02	6.68E+02
SierradeSegura	1.73E+02	6.68E+02
SierraMorena	1.73E+02	6.68E+02
SierraRiojaAlta	1.47E+02	4.24E+02
SierraRiojaBaja	1.47E+02	4.24E+02
SierraRiojaMedia	1.47E+02	4.24E+02
SierraSegura	7.40E+01	4.63E+02
SierraSur	1.73E+02	6.68E+02
Sobrado	2.61E+02	2.66E+02
Sobrarbe	8.00E+01	3.88E+02
Solsones	1.74E+02	4.26E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
Somontano	8.00E+01	3.88E+02
Somozas	2.61E+02	2.66E+02
Soria	1.29E+02	3.67E+02
Sur	2.61E+02	2.66E+02
Sur	1.29E+02	3.67E+02
SurdeTenerife	1.67E+03	3.82E+03
SurOcci-dental	4.90E+01	3.46E+02
Sureste	1.29E+02	3.67E+02
SuroesteyValleGuadalentin	1.13E+02	7.74E+02
Talavera	7.40E+01	4.63E+02
TerraAlta	1.74E+02	4.26E+02
TerraCha	2.61E+02	2.66E+02
TierradeCampos	1.29E+02	3.67E+02
TierraEstella	1.95E+02	3.80E+02
TierrasAltasyValledelTera	1.29E+02	3.67E+02
TierrasdeLeon	1.29E+02	3.67E+02
Toques	2.61E+02	2.66E+02
Tordoia	2.61E+02	2.66E+02
Torrijos	7.40E+01	4.63E+02
Touro	2.61E+02	2.66E+02
Trazo	2.61E+02	2.66E+02
Trujillo	7.90E+01	5.42E+02
Tudanca-Cabuerniga	2.08E+02	1.00E+05
Urgel	1.74E+02	4.26E+02
ValdoDubra	2.61E+02	2.66E+02
ValenciadeAlcantara	7.90E+01	5.42E+02
ValledeAran	1.74E+02	4.26E+02
ValledeAyora	5.70E+01	7.32E+02
ValledeLecrin	1.73E+02	6.68E+02
ValledelBajoAlberche	1.29E+02	3.67E+02
ValledelTietar	1.29E+02	3.67E+02

Table D.9: .-Land rental price (€/ha) (Junta de Castilla y León, 2019)

Region	Rainfed	Irrigate
VallesAlaveses	2.37E+02	1.00E+05
VallesdeAlbaida	5.70E+01	7.32E+02
VallesOccidental	1.74E+02	4.26E+02
VallesOriental	1.74E+02	4.26E+02
Vegadeo	1.78E+02	1.00E+05
Vegas	4.90E+01	3.46E+02
Velez-Malaga	1.73E+02	6.68E+02
Verin	2.61E+02	2.66E+02
Vilasantar	2.61E+02	2.66E+02
Vinalopo	5.70E+01	7.32E+02
Vitigudino	1.29E+02	3.67E+02
Vizcaya	1.29E+02	1.00E+05
Zaragoza	8.00E+01	3.88E+02

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
1	4.6E+02	3.9E+02	2.0E+03	0.0E+00	0.0E+00	0.0E+00	2.6E+02	1.7E+03	2.6E+02	3.6E+01
2	1.2E+00	8.4E+02	4.5E+03	0.0E+00	0.0E+00	2.6E+00	1.1E+03	6.6E+03	1.1E+03	3.6E+03
3	0.0E+00	5.0E+02	2.1E+03	0.0E+00	0.0E+00	0.0E+00	1.8E+00	2.3E+03	1.8E+00	1.0E+03
4	8.0E+00	4.4E+01	4.4E+04	0.0E+00	4.5E+00	6.7E-01	1.1E+02	5.1E+03	1.1E+02	1.5E+01
5	2.1E+02	2.2E+02	2.6E+04	0.0E+00	2.9E+00	0.0E+00	1.0E+03	1.5E+04	1.0E+03	7.4E+01
6	5.0E+01	5.3E+01	6.3E+03	0.0E+00	7.0E-01	0.0E+00	2.4E+02	3.6E+03	2.4E+02	1.8E+01
7	5.8E+00	1.9E+01	4.2E+03	0.0E+00	3.6E+00	5.5E-01	4.5E+01	1.3E+03	4.5E+01	5.9E+01
8	9.6E+02	1.2E+03	4.9E+03	0.0E+00	0.0E+00	0.0E+00	3.6E+02	4.8E+03	3.6E+02	2.3E+03
9	0.0E+00	1.3E+01	7.9E+03	0.0E+00	0.0E+00	0.0E+00	1.8E+02	3.3E+03	1.8E+02	2.1E+01
10	1.8E+02	7.1E+02	1.7E+04	0.0E+00	0.0E+00	0.0E+00	3.7E+03	1.9E+04	3.7E+03	0.0E+00
11	0.0E+00	1.3E+03	5.3E+03	0.0E+00	0.0E+00	0.0E+00	4.5E+00	6.0E+03	4.5E+00	2.6E+03
12	0.0E+00	2.0E+00	9.5E+02	0.0E+00	1.1E-01	1.1E-01	2.0E+01	3.7E+02	2.0E+01	1.7E+02
13	1.7E+03	8.7E+00	4.9E+03	4.5E+02	3.2E+02	1.3E+02	1.1E+02	2.4E+03	1.1E+02	2.2E+03
14	0.0E+00	2.9E-02	1.4E+01	0.0E+00	1.5E-03	1.5E-03	2.9E-01	5.3E+00	2.9E-01	2.5E+00
15	8.6E+01	1.2E+01	1.4E+03	1.4E+01	3.6E+01	1.0E+01	1.6E+02	3.3E+02	1.6E+02	7.2E+01
16	1.3E+01	6.7E+00	1.3E+03	0.0E+00	0.0E+00	0.0E+00	1.3E+01	3.9E+02	1.3E+01	0.0E+00
17	4.7E+01	4.1E-01	1.2E+03	3.7E-01	2.5E+00	2.3E-01	5.6E+00	5.3E+02	5.6E+00	9.7E+01
18	1.4E+01	3.0E+01	1.8E+02	0.0E+00	3.3E+00	3.4E-01	8.0E-01	1.5E+03	8.0E-01	2.8E+02
19	1.9E+00	4.1E+00	2.5E+01	0.0E+00	4.5E-01	4.7E-02	1.1E-01	2.1E+02	1.1E-01	3.9E+01
20	7.8E+02	0.0E+00	8.8E+03	3.0E+02	3.9E+01	0.0E+00	5.4E+00	4.3E+03	5.4E+00	1.6E+03
21	3.5E+01	1.5E+03	8.5E+03	0.0E+00	2.1E+00	0.0E+00	0.0E+00	1.1E+04	0.0E+00	1.2E+03
22	7.6E+00	1.4E+01	4.8E+00	1.3E+03	2.0E+02	0.0E+00	2.5E+00	5.6E+01	2.5E+00	6.5E+00

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
23	8.8E+01	3.5E+02	8.3E+03	0.0E+00	0.0E+00	0.0E+00	1.8E+03	9.1E+03	1.8E+03	0.0E+00
24	6.3E+00	0.0E+00	7.5E+03	0.0E+00	6.2E+01	4.6E-01	2.3E+02	2.1E+03	2.3E+02	1.8E+01
25	4.4E+00	3.6E+03	3.6E+04	0.0E+00	0.0E+00	0.0E+00	9.3E+03	2.3E+04	9.3E+03	3.7E+03
26	1.2E+03	2.8E+03	3.0E+04	1.1E+01	0.0E+00	0.0E+00	1.1E+03	4.2E+04	1.1E+03	2.8E+01
27	9.9E+02	2.4E+03	2.6E+04	9.7E+00	0.0E+00	0.0E+00	9.7E+02	3.6E+04	9.7E+02	2.3E+01
28	1.9E+01	3.5E+01	1.2E+01	3.3E+03	5.0E+02	0.0E+00	6.2E+00	1.4E+02	6.2E+00	1.6E+01
29	3.3E+00	5.5E+00	3.6E+00	2.4E+01	2.7E-01	1.1E-01	1.2E+00	1.5E+01	1.2E+00	1.4E+00
30	3.3E+02	6.8E+02	1.2E+03	0.0E+00	0.0E+00	0.0E+00	6.7E+02	2.0E+03	6.7E+02	1.4E+02
31	1.4E+00	1.2E+03	1.2E+04	0.0E+00	0.0E+00	0.0E+00	3.0E+03	7.3E+03	3.0E+03	1.2E+03
32	0.0E+00	2.5E+03	1.0E+04	0.0E+00	0.0E+00	0.0E+00	8.7E+00	1.2E+04	8.7E+00	5.0E+03
33	0.0E+00	1.8E+03	7.2E+03	0.0E+00	0.0E+00	0.0E+00	6.2E+00	8.2E+03	6.2E+00	3.5E+03
34	5.6E+02	0.0E+00	6.3E+03	2.1E+02	2.8E+01	0.0E+00	3.8E+00	3.1E+03	3.8E+00	1.2E+03
35	0.0E+00	1.1E+00	5.2E+02	0.0E+00	5.8E-02	5.8E-02	1.1E+01	2.0E+02	1.1E+01	9.4E+01
36	9.7E+02	5.0E+00	2.8E+03	2.6E+02	1.8E+02	7.6E+01	6.2E+01	1.4E+03	6.2E+01	1.3E+03
37	0.0E+00	9.7E+01	2.3E+04	3.1E+01	0.0E+00	0.0E+00	2.1E+03	7.3E+03	2.1E+03	1.9E+01
38	5.9E+02	2.1E+02	1.4E+04	0.0E+00	0.0E+00	1.6E+01	9.8E+01	6.5E+03	9.8E+01	5.1E+00
39	8.1E+00	0.0E+00	8.2E+02	0.0E+00	5.6E-02	1.1E-01	3.4E-01	3.1E+02	3.4E-01	9.1E+01
40	1.5E+01	0.0E+00	1.7E+02	5.7E+00	7.4E-01	0.0E+00	1.0E-01	8.2E+01	1.0E-01	3.1E+01
41	1.2E+01	1.6E+00	1.9E+02	1.9E+00	4.8E+00	1.3E+00	2.1E+01	4.4E+01	2.1E+01	9.6E+00
42	3.0E+00	0.0E+00	3.1E+02	0.0E+00	2.1E-02	4.2E-02	1.3E-01	1.2E+02	1.3E-01	3.4E+01
43	7.3E-02	6.0E+01	5.9E+02	0.0E+00	0.0E+00	0.0E+00	1.5E+02	3.7E+02	1.5E+02	6.1E+01
44	8.0E+00	2.6E+01	5.7E+03	0.0E+00	5.0E+00	7.5E-01	6.1E+01	1.8E+03	6.1E+01	8.1E+01
45	6.7E-01	0.0E+00	0.0E+00	8.3E+01	5.1E+00	0.0E+00	0.0E+00	7.6E-01	0.0E+00	0.0E+00
46	1.1E+03	1.4E+03	5.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+02	5.5E+03	4.2E+02	2.6E+03
47	2.8E+02	0.0E+00	3.2E+03	1.1E+02	1.4E+01	0.0E+00	2.0E+00	1.6E+03	2.0E+00	5.9E+02
48	8.8E+00	1.8E+01	3.2E+01	0.0E+00	0.0E+00	0.0E+00	1.8E+01	5.2E+01	1.8E+01	3.8E+00
49	2.1E+03	1.8E+03	9.0E+03	0.0E+00	0.0E+00	0.0E+00	1.2E+03	7.4E+03	1.2E+03	1.6E+02
50	9.9E+00	1.9E+01	6.2E+00	1.8E+03	2.7E+02	0.0E+00	3.3E+00	7.3E+01	3.3E+00	8.5E+00
51	8.5E+01	8.9E+00	7.4E+03	0.0E+00	2.9E+00	5.6E-01	1.6E+02	4.5E+03	1.6E+02	2.5E+00
52	0.0E+00	2.3E+02	4.5E+01	0.0E+00	0.0E+00	0.0E+00	1.9E+00	1.9E+02	1.9E+00	4.1E+02
53	9.8E+02	2.4E+03	2.6E+04	9.6E+00	0.0E+00	0.0E+00	9.7E+02	3.6E+04	9.7E+02	2.3E+01
54	1.6E+02	6.5E+02	1.6E+04	0.0E+00	0.0E+00	0.0E+00	3.3E+03	1.7E+04	3.3E+03	0.0E+00
55	0.0E+00	7.7E+02	1.5E+02	0.0E+00	0.0E+00	0.0E+00	6.3E+00	6.4E+02	6.3E+00	1.4E+03
56	2.0E+02	2.1E+01	1.7E+04	0.0E+00	6.7E+00	1.3E+00	3.8E+02	1.0E+04	3.8E+02	5.8E+00
57	1.5E+01	0.0E+00	1.8E+04	0.0E+00	1.5E+02	1.1E+00	5.7E+02	5.2E+03	5.7E+02	4.5E+01
58	2.4E+02	2.6E+02	3.1E+04	0.0E+00	3.4E+00	0.0E+00	1.2E+03	1.8E+04	1.2E+03	8.6E+01
59	1.3E+00	7.2E+00	1.4E+03	0.0E+00	5.7E-01	3.2E+00	2.4E+01	3.5E+03	2.4E+01	2.6E+02
60	8.2E+00	4.6E+01	9.1E+03	0.0E+00	3.6E+00	2.0E+01	1.5E+02	2.2E+04	1.5E+02	1.6E+03
61	9.5E+01	3.2E+00	7.0E+03	0.0E+00	3.7E+01	1.2E+03	3.2E+00	3.3E+04	3.2E+00	4.2E+03
62	5.7E+00	3.3E+01	1.6E+03	4.6E-01	0.0E+00	0.0E+00	1.2E+01	1.2E+03	1.2E+01	1.6E+02
63	2.9E+00	1.6E+01	8.3E+02	2.3E-01	0.0E+00	0.0E+00	6.2E+00	5.9E+02	6.2E+00	8.0E+01
64	0.0E+00	9.9E-03	4.7E+00	0.0E+00	5.2E-04	5.2E-04	9.9E-02	1.8E+00	9.9E-02	8.4E-01
65	0.0E+00	7.8E+02	2.1E+04	0.0E+00	8.1E+00	7.4E+00	3.2E+02	7.0E+03	3.2E+02	3.9E+02
66	0.0E+00	4.4E+00	7.6E+02	7.0E-02	3.1E-01	7.3E-01	4.5E+00	3.0E+02	4.5E+00	2.5E-01
67	5.8E+00	1.9E-01	4.2E+02	0.0E+00	2.2E+00	7.2E+01	1.9E-01	2.0E+03	1.9E-01	2.5E+02
68	0.0E+00	8.5E+02	2.3E+04	0.0E+00	8.9E+00	8.0E+00	3.5E+02	7.6E+03	3.5E+02	4.2E+02
69	1.7E+01	0.0E+00	1.7E+03	0.0E+00	1.2E-01	2.3E-01	7.0E-01	6.4E+02	7.0E-01	1.9E+02
70	0.0E+00	1.4E-01	6.8E+01	0.0E+00	7.5E-03	7.5E-03	1.4E+00	2.6E+01	1.4E+00	1.2E+01
71	0.0E+00	1.8E+00	8.6E+02	0.0E+00	9.5E-02	9.5E-02	1.8E+01	3.3E+02	1.8E+01	1.5E+02
72	1.4E+04	1.2E+04	6.1E+04	0.0E+00	0.0E+00	0.0E+00	7.9E+03	5.0E+04	7.9E+03	1.1E+03
73	3.3E+02	1.3E+03	3.1E+04	0.0E+00	0.0E+00	0.0E+00	6.6E+03	3.4E+04	6.6E+03	0.0E+00

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
74	9.9E-01	5.3E-01	1.0E+02	0.0E+00	0.0E+00	0.0E+00	1.0E+00	3.1E+01	1.0E+00	0.0E+00
75	4.8E+03	6.0E+03	2.4E+04	0.0E+00	0.0E+00	0.0E+00	1.8E+03	2.4E+04	1.8E+03	1.1E+04
76	8.7E+00	0.0E+00	0.0E+00	1.1E+03	6.6E+01	0.0E+00	0.0E+00	9.9E+00	0.0E+00	0.0E+00
77	1.1E+00	0.0E+00	0.0E+00	1.4E+02	8.4E+00	0.0E+00	0.0E+00	1.3E+00	0.0E+00	0.0E+00
78	1.2E+01	3.1E+01	3.9E+02	7.2E-01	1.1E-01	0.0E+00	2.9E+00	6.9E+02	2.9E+00	4.3E-01
79	2.1E+00	3.9E+00	1.3E+00	3.7E+02	5.6E+01	0.0E+00	6.9E-01	1.5E+01	6.9E-01	1.8E+00
80	1.7E+02	1.8E+01	1.5E+04	0.0E+00	5.9E+00	1.1E+00	3.3E+02	9.2E+03	3.3E+02	5.1E+00
81	0.0E+00	1.5E+03	5.9E+03	0.0E+00	0.0E+00	0.0E+00	5.1E+00	6.7E+03	5.1E+00	2.9E+03
82	1.6E+01	7.1E+01	8.8E+00	7.5E+03	8.1E+02	0.0E+00	2.0E+02	1.2E+03	2.0E+02	1.6E+02
83	3.5E-01	9.8E-01	1.6E+02	0.0E+00	7.0E-02	4.2E-01	4.8E+00	6.3E+01	4.8E+00	7.0E-02
84	6.4E+03	4.4E+03	5.2E+04	0.0E+00	0.0E+00	0.0E+00	2.6E+03	2.7E+04	2.6E+03	3.5E+02
85	0.0E+00	6.0E+01	3.8E+04	0.0E+00	0.0E+00	0.0E+00	8.7E+02	1.6E+04	8.7E+02	9.9E+01
86	0.0E+00	8.4E+00	1.5E+03	1.3E-01	6.1E-01	1.4E+00	8.7E+00	5.8E+02	8.7E+00	4.7E-01
87	1.6E+01	3.0E+01	9.9E+00	2.8E+03	4.2E+02	0.0E+00	5.3E+00	1.2E+02	5.3E+00	1.4E+01
88	1.1E+02	5.7E-01	3.3E+02	3.0E+01	2.1E+01	8.7E+00	7.1E+00	1.6E+02	7.1E+00	1.5E+02
89	3.5E+02	3.0E+02	1.5E+03	0.0E+00	0.0E+00	0.0E+00	2.0E+02	1.2E+03	2.0E+02	2.7E+01
90	6.0E-01	4.4E+02	2.4E+03	0.0E+00	0.0E+00	1.3E+00	5.8E+02	3.5E+03	5.8E+02	1.9E+03
91	2.4E+02	2.1E+00	6.0E+03	1.9E+00	1.3E+01	1.2E+00	2.9E+01	2.7E+03	2.9E+01	4.9E+02
92	2.9E+01	0.0E+00	2.9E+03	0.0E+00	2.0E-01	4.0E-01	1.2E+00	1.1E+03	1.2E+00	3.3E+02
93	7.3E+01	1.6E+02	9.6E+02	0.0E+00	1.8E+01	1.8E+00	4.2E+00	8.1E+03	4.2E+00	1.5E+03
94	8.0E+00	1.7E+01	1.1E+02	0.0E+00	1.9E+00	2.0E-01	4.7E-01	8.9E+02	4.7E-01	1.7E+02
95	0.0E+00	8.1E+02	1.6E+02	0.0E+00	0.0E+00	0.0E+00	6.6E+00	6.7E+02	6.6E+00	1.5E+03
96	2.0E+00	9.0E+00	1.1E+00	9.5E+02	1.0E+02	0.0E+00	2.5E+01	1.5E+02	2.5E+01	2.0E+01
97	1.9E+01	4.1E+01	2.5E+02	0.0E+00	4.6E+00	4.7E-01	1.1E+00	2.1E+03	1.1E+00	4.0E+02
98	1.2E+01	4.0E-01	8.7E+02	0.0E+00	4.6E+00	1.5E+02	4.0E-01	4.1E+03	4.0E-01	5.2E+02
99	9.3E+01	1.6E+02	1.0E+02	6.9E+02	7.7E+00	3.2E+00	3.4E+01	4.1E+02	3.4E+01	3.9E+01
100	0.0E+00	1.3E+03	3.9E+04	0.0E+00	0.0E+00	1.2E+01	6.4E+03	3.8E+04	6.4E+03	1.2E+03
101	0.0E+00	1.1E+02	2.5E+04	3.4E+01	0.0E+00	0.0E+00	2.3E+03	8.0E+03	2.3E+03	2.1E+01
102	7.4E+01	7.9E+02	1.0E+04	2.3E+02	1.6E-01	0.0E+00	1.5E+01	1.1E+04	1.5E+01	9.9E+01
103	7.4E+00	1.4E+01	4.7E+00	1.3E+03	2.0E+02	0.0E+00	2.5E+00	5.4E+01	2.5E+00	6.4E+00
104	2.7E+02	2.8E+01	2.3E+04	0.0E+00	9.1E+00	1.8E+00	5.1E+02	1.4E+04	5.1E+02	7.9E+00
105	2.1E+00	1.8E+01	5.7E+02	1.2E-01	1.1E+00	3.3E+00	0.0E+00	2.3E+03	0.0E+00	1.3E+02
106	2.5E+01	8.3E-01	1.8E+03	0.0E+00	9.6E+00	3.1E+02	8.3E-01	8.5E+03	8.3E-01	1.1E+03
107	4.1E+00	1.4E+01	3.0E+03	0.0E+00	2.6E+00	3.9E-01	3.2E+01	9.5E+02	3.2E+01	4.2E+01
108	1.5E+02	3.6E+02	3.9E+03	1.5E+00	0.0E+00	0.0E+00	1.5E+02	5.4E+03	1.5E+02	3.5E+00
109	0.0E+00	1.3E+03	5.4E+03	0.0E+00	0.0E+00	0.0E+00	4.6E+00	6.1E+03	4.6E+00	2.6E+03
110	3.2E+03	4.0E+03	1.6E+04	0.0E+00	0.0E+00	0.0E+00	1.2E+03	1.6E+04	1.2E+03	7.5E+03
111	3.2E+02	3.3E+01	2.8E+04	0.0E+00	1.1E+01	2.1E+00	6.1E+02	1.7E+04	6.1E+02	9.4E+00
112	5.2E+00	4.6E+01	1.4E+03	3.1E-01	2.7E+00	8.3E+00	0.0E+00	5.8E+03	0.0E+00	3.3E+02
113	1.1E+00	2.8E+00	6.3E+01	7.3E+01	1.9E+02	0.0E+00	4.2E+02	7.7E+02	4.2E+02	1.9E+01
114	6.2E+03	5.3E+03	2.7E+04	0.0E+00	0.0E+00	0.0E+00	3.5E+03	2.2E+04	3.5E+03	4.9E+02
115	1.7E+00	9.6E+00	4.8E+02	1.3E-01	0.0E+00	0.0E+00	3.6E+00	3.5E+02	3.6E+00	4.7E+01
116	2.6E+02	5.2E+02	9.3E+02	0.0E+00	0.0E+00	0.0E+00	5.1E+02	1.5E+03	5.1E+02	1.1E+02
117	8.3E-01	4.4E-01	8.4E+01	0.0E+00	0.0E+00	0.0E+00	8.7E-01	2.6E+01	8.7E-01	0.0E+00
118	1.9E+03	3.9E+03	7.0E+03	0.0E+00	0.0E+00	0.0E+00	3.9E+03	1.2E+04	3.9E+03	8.2E+02
119	1.9E+01	4.9E+01	6.3E+02	1.2E+00	1.8E-01	0.0E+00	4.6E+00	1.1E+03	4.6E+00	6.9E-01
120	1.2E+01	2.2E+01	7.3E+00	2.1E+03	3.1E+02	0.0E+00	3.9E+00	8.5E+01	3.9E+00	1.0E+01
121	7.3E-01	5.4E+02	2.9E+03	0.0E+00	0.0E+00	1.6E+00	7.1E+02	4.2E+03	7.1E+02	2.3E+03
122	2.7E+00	0.0E+00	2.0E+01	3.6E+01	3.2E+01	0.0E+00	1.5E+01	2.2E+01	1.5E+01	8.9E+01
123	4.9E-03	2.6E-03	5.0E-01	0.0E+00	0.0E+00	0.0E+00	5.2E-03	1.5E-01	5.2E-03	0.0E+00
124	1.6E+02	1.4E+00	4.0E+03	1.2E+00	8.2E+00	7.7E-01	1.9E+01	1.8E+03	1.9E+01	3.2E+02

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
125	6.5E+02	3.3E+00	1.9E+03	1.7E+02	1.2E+02	5.1E+01	4.1E+01	9.1E+02	4.1E+01	8.6E+02
126	6.5E+00	0.0E+00	0.0E+00	8.1E+02	4.9E+01	0.0E+00	0.0E+00	7.5E+00	0.0E+00	0.0E+00
127	1.4E+03	7.3E+00	4.2E+03	3.8E+02	2.7E+02	1.1E+02	9.1E+01	2.0E+03	9.1E+01	1.9E+03
128	6.0E+00	0.0E+00	0.0E+00	7.5E+02	4.6E+01	0.0E+00	0.0E+00	6.9E+00	0.0E+00	0.0E+00
129	3.6E+00	0.0E+00	2.6E+01	4.7E+01	4.2E+01	0.0E+00	1.9E+01	2.8E+01	1.9E+01	1.2E+02
130	2.5E-03	2.0E+00	2.0E+01	0.0E+00	0.0E+00	0.0E+00	5.2E+00	1.3E+01	5.2E+00	2.1E+00
131	6.9E+00	2.9E+02	1.7E+03	0.0E+00	4.2E-01	0.0E+00	0.0E+00	2.2E+03	0.0E+00	2.3E+02
132	2.7E-02	0.0E+00	3.1E+01	0.0E+00	2.6E-01	1.9E-03	9.7E-01	8.9E+00	9.7E-01	7.7E-02
133	6.7E+00	2.2E+01	4.7E+03	0.0E+00	4.1E+00	6.3E-01	5.1E+01	1.5E+03	5.1E+01	6.8E+01
134	4.3E+02	3.7E+02	1.9E+03	0.0E+00	0.0E+00	0.0E+00	2.4E+02	1.6E+03	2.4E+02	3.4E+01
135	5.0E+01	4.0E+01	0.0E+00	1.8E+02	1.0E+02	0.0E+00	0.0E+00	3.0E+00	0.0E+00	1.5E+01
136	0.0E+00	6.6E+00	4.1E+03	0.0E+00	0.0E+00	0.0E+00	9.6E+01	1.7E+03	9.6E+01	1.1E+01
137	0.0E+00	1.8E+02	7.5E+02	0.0E+00	0.0E+00	0.0E+00	6.5E-01	8.5E+02	6.5E-01	3.7E+02
138	0.0E+00	7.2E+01	1.4E+01	0.0E+00	0.0E+00	0.0E+00	5.9E-01	6.0E+01	5.9E-01	1.3E+02
139	1.0E+00	5.4E-01	1.0E+02	0.0E+00	0.0E+00	0.0E+00	1.1E+00	3.2E+01	1.1E+00	0.0E+00
140	2.0E+03	6.8E+02	4.7E+04	0.0E+00	0.0E+00	5.1E+01	3.3E+02	2.2E+04	3.3E+02	1.7E+01
141	0.0E+00	7.9E+01	1.9E+04	2.5E+01	0.0E+00	0.0E+00	1.7E+03	5.9E+03	1.7E+03	1.6E+01
142	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
143	1.3E+01	4.2E+01	9.1E+03	0.0E+00	8.0E+00	1.2E+00	9.8E+01	2.9E+03	9.8E+01	1.3E+02
144	0.0E+00	1.6E+01	1.4E+03	0.0E+00	0.0E+00	0.0E+00	3.5E-01	4.1E+02	3.5E-01	1.3E+02
145	0.0E+00	1.4E+00	5.0E-01	2.5E+02	2.5E+02	0.0E+00	2.0E-01	8.3E+00	2.0E-01	4.6E+00
146	4.3E+00	8.2E+00	2.7E+00	7.7E+02	1.2E+02	0.0E+00	1.5E+00	3.2E+01	1.5E+00	3.7E+00
147	0.0E+00	1.2E-01	1.0E-01	2.2E-01	2.8E-01	0.0E+00	1.3E-01	3.5E-01	1.3E-01	8.9E-01
148	0.0E+00	2.4E+00	2.0E+00	4.4E+00	5.4E+00	0.0E+00	2.5E+00	6.7E+00	2.5E+00	1.7E+01
149	0.0E+00	8.1E+00	6.5E+00	1.5E+01	1.8E+01	0.0E+00	8.4E+00	2.3E+01	8.4E+00	5.8E+01
150	1.3E+01	4.2E+01	9.1E+03	0.0E+00	7.9E+00	1.2E+00	9.8E+01	2.9E+03	9.8E+01	1.3E+02
151	4.4E+02	1.5E+02	1.0E+04	0.0E+00	0.0E+00	1.2E+01	7.3E+01	4.8E+03	7.3E+01	3.8E+00
152	0.0E+00	4.7E+01	9.3E+00	0.0E+00	0.0E+00	0.0E+00	3.9E-01	4.0E+01	3.9E-01	8.6E+01
153	0.0E+00	3.2E+02	1.3E+03	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.5E+03	1.1E+00	6.3E+02
154	1.6E+02	1.7E+01	1.4E+04	0.0E+00	5.5E+00	1.1E+00	3.1E+02	8.6E+03	3.1E+02	4.8E+00
155	1.9E+02	4.0E+02	7.0E+02	0.0E+00	0.0E+00	0.0E+00	3.9E+02	1.2E+03	3.9E+02	8.3E+01
156	6.2E+01	1.3E+02	2.2E+02	0.0E+00	0.0E+00	0.0E+00	1.2E+02	3.7E+02	1.2E+02	2.6E+01
157	7.3E+01	6.4E+02	2.0E+04	4.3E+00	3.8E+01	1.2E+02	0.0E+00	8.1E+04	0.0E+00	4.6E+03
158	1.9E-02	6.2E-02	1.3E+01	0.0E+00	1.2E-02	1.8E-03	1.4E-01	4.3E+00	1.4E-01	1.9E-01
159	6.4E+00	3.4E+00	6.5E+02	0.0E+00	0.0E+00	0.0E+00	6.7E+00	2.0E+02	6.7E+00	0.0E+00
160	1.5E+01	3.3E+02	1.1E+04	0.0E+00	0.0E+00	3.9E-01	6.6E+02	3.5E+03	6.6E+02	6.9E+02
161	3.0E+02	1.1E+02	7.2E+03	0.0E+00	0.0E+00	7.9E+00	5.0E+01	3.3E+03	5.0E+01	2.6E+00
162	2.9E+00	1.7E+01	8.3E+02	2.3E-01	0.0E+00	0.0E+00	6.3E+00	6.0E+02	6.3E+00	8.1E+01
163	6.8E+01	1.4E+03	4.7E+04	0.0E+00	0.0E+00	1.7E+00	2.9E+03	1.5E+04	2.9E+03	3.1E+03
164	5.5E+00	1.1E+01	2.0E+01	0.0E+00	0.0E+00	0.0E+00	1.1E+01	3.3E+01	1.1E+01	2.4E+00
165	2.1E+01	4.2E+01	7.5E+01	0.0E+00	0.0E+00	0.0E+00	4.2E+01	1.2E+02	4.2E+01	8.8E+00
166	4.2E+00	5.9E-01	6.8E+01	6.7E-01	1.7E+00	4.8E-01	7.6E+00	1.6E+01	7.6E+00	3.5E+00
167	6.4E+02	1.5E+03	1.7E+04	6.2E+00	0.0E+00	0.0E+00	6.3E+02	2.3E+04	6.3E+02	1.5E+01
168	5.3E+02	2.8E+00	1.6E+03	1.4E+02	1.0E+02	4.2E+01	3.4E+01	7.5E+02	3.4E+01	7.1E+02
169	2.0E-02	1.5E+01	8.0E+01	0.0E+00	0.0E+00	4.5E-02	2.0E+01	1.2E+02	2.0E+01	6.4E+01
170	7.1E-01	4.0E+00	8.0E+02	0.0E+00	3.2E-01	1.8E+00	1.3E+01	2.0E+03	1.3E+01	1.4E+02
171	6.0E+00	5.3E+01	1.6E+03	3.6E-01	3.1E+00	9.5E+00	0.0E+00	6.7E+03	0.0E+00	3.7E+02
172	8.5E+00	7.5E+01	2.3E+03	5.0E-01	4.5E+00	1.3E+01	0.0E+00	9.5E+03	0.0E+00	5.3E+02
173	2.9E+00	2.5E+01	7.9E+02	1.7E-01	1.5E+00	4.5E+00	0.0E+00	3.2E+03	0.0E+00	1.8E+02
174	7.7E+00	0.0E+00	5.5E+01	1.0E+02	9.0E+01	0.0E+00	4.1E+01	6.1E+01	4.1E+01	2.5E+02
175	2.7E-02	9.0E-02	1.9E+01	0.0E+00	1.7E-02	2.6E-03	2.1E-01	6.2E+00	2.1E-01	2.8E-01

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
176	8.9E-01	5.0E+00	1.0E+03	0.0E+00	4.0E-01	2.2E+00	1.6E+01	2.5E+03	1.6E+01	1.8E+02
177	3.5E+00	3.1E+01	9.7E+02	2.1E-01	1.9E+00	5.6E+00	0.0E+00	4.0E+03	0.0E+00	2.2E+02
178	5.7E-01	4.2E+02	2.3E+03	0.0E+00	0.0E+00	1.3E+00	5.5E+02	3.3E+03	5.5E+02	1.8E+03
179	1.4E+00	2.4E+00	1.5E+00	1.0E+01	1.2E-01	4.8E-02	5.1E-01	6.2E+00	5.1E-01	5.8E-01
180	0.0E+00	5.2E+00	1.8E+00	9.3E+02	9.3E+02	0.0E+00	7.4E-01	3.1E+01	7.4E-01	1.7E+01
181	9.3E-01	1.3E-01	1.5E+01	1.5E-01	3.8E-01	1.1E-01	1.7E+00	3.6E+00	1.7E+00	7.7E-01
182	1.8E+02	4.7E+02	6.0E+03	1.1E+01	1.8E+00	0.0E+00	4.4E+01	1.1E+04	4.4E+01	6.6E+00
183	5.0E+00	0.0E+00	0.0E+00	6.3E+02	3.8E+01	0.0E+00	0.0E+00	5.8E+00	0.0E+00	0.0E+00
184	2.9E+01	4.1E+00	4.8E+02	4.7E+00	1.2E+01	3.4E+00	5.3E+01	1.1E+02	5.3E+01	2.4E+01
185	0.0E+00	2.0E+03	8.2E+03	0.0E+00	0.0E+00	0.0E+00	7.1E+00	9.3E+03	7.1E+00	4.0E+03
186	0.0E+00	7.7E+02	1.5E+02	0.0E+00	0.0E+00	0.0E+00	6.3E+00	6.4E+02	6.3E+00	1.4E+03
187	0.0E+00	1.4E+01	6.6E+03	0.0E+00	7.3E-01	7.3E-01	1.4E+02	2.5E+03	1.4E+02	1.2E+03
188	1.7E+00	0.0E+00	2.1E+03	0.0E+00	1.7E+01	1.3E-01	6.4E+01	5.9E+02	6.4E+01	5.0E+00
189	1.9E+01	0.0E+00	0.0E+00	2.3E+03	1.4E+02	0.0E+00	0.0E+00	2.1E+01	0.0E+00	0.0E+00
190	0.0E+00	2.3E+01	5.4E+03	7.3E+00	0.0E+00	0.0E+00	4.9E+02	1.7E+03	4.9E+02	4.6E+00
191	3.8E+00	2.2E+01	1.1E+03	3.0E-01	0.0E+00	0.0E+00	8.2E+00	7.9E+02	8.2E+00	1.1E+02
192	0.0E+00	1.3E+02	1.2E+04	0.0E+00	0.0E+00	0.0E+00	3.0E+00	3.5E+03	3.0E+00	1.1E+03
193	0.0E+00	2.1E+01	1.3E+04	0.0E+00	0.0E+00	0.0E+00	3.0E+02	5.4E+03	3.0E+02	3.4E+01
194	0.0E+00	5.8E+01	3.7E+04	0.0E+00	0.0E+00	0.0E+00	8.5E+02	1.5E+04	8.5E+02	9.7E+01
195	0.0E+00	8.7E+02	2.3E+04	0.0E+00	9.2E+00	8.3E+00	3.6E+02	7.9E+03	3.6E+02	4.4E+02
196	1.8E+01	9.7E+01	9.5E+04	0.0E+00	9.9E+00	1.5E+00	2.4E+02	1.1E+04	2.4E+02	3.4E+01
197	8.3E+00	4.6E+01	4.5E+04	0.0E+00	4.7E+00	7.0E-01	1.1E+02	5.3E+03	1.1E+02	1.6E+01
198	6.5E+00	3.6E+01	3.5E+04	0.0E+00	3.6E+00	5.4E-01	8.8E+01	4.1E+03	8.8E+01	1.2E+01
199	1.7E+01	0.0E+00	2.0E+02	6.6E+00	8.6E-01	0.0E+00	1.2E-01	9.6E+01	1.2E-01	3.6E+01
200	2.7E-03	7.5E-03	1.2E+00	0.0E+00	5.4E-04	3.2E-03	3.7E-02	4.8E-01	3.7E-02	5.4E-04
201	4.9E+00	9.1E+00	3.1E+00	8.6E+02	1.3E+02	0.0E+00	1.6E+00	3.6E+01	1.6E+00	4.2E+00
202	0.0E+00	7.6E+01	6.9E+03	0.0E+00	0.0E+00	0.0E+00	1.7E+00	2.0E+03	1.7E+00	6.1E+02
203	0.0E+00	1.4E+03	5.9E+03	0.0E+00	0.0E+00	0.0E+00	5.1E+00	6.7E+03	5.1E+00	2.9E+03
204	1.1E-01	3.1E-01	5.1E+01	0.0E+00	2.2E-02	1.3E-01	1.5E+00	2.0E+01	1.5E+00	2.2E-02
205	3.6E+02	8.7E+02	9.5E+03	3.6E+00	0.0E+00	0.0E+00	3.6E+02	1.3E+04	3.6E+02	8.6E+00
206	1.5E+01	2.9E+01	9.6E+00	2.7E+03	4.1E+02	0.0E+00	5.1E+00	1.1E+02	5.1E+00	1.3E+01
207	7.7E-01	0.0E+00	0.0E+00	9.6E+01	5.8E+00	0.0E+00	0.0E+00	8.8E-01	0.0E+00	0.0E+00
208	0.0E+00	2.2E+00	7.8E-01	3.9E+02	3.9E+02	0.0E+00	3.1E-01	1.3E+01	3.1E-01	7.2E+00
209	1.9E+02	2.0E+02	2.4E+04	0.0E+00	2.7E+00	0.0E+00	9.3E+02	1.4E+04	9.3E+02	6.8E+01
210	5.3E+02	1.9E+02	1.3E+04	0.0E+00	0.0E+00	1.4E+01	8.9E+01	5.9E+03	8.9E+01	4.6E+00
211	6.1E+00	1.2E+01	3.9E+00	1.1E+03	1.6E+02	0.0E+00	2.1E+00	4.5E+01	2.1E+00	5.3E+00
212	3.6E+00	1.6E+01	2.0E+00	1.7E+03	1.9E+02	0.0E+00	4.6E+01	2.7E+02	4.6E+01	3.6E+01
213	0.0E+00	1.9E+01	6.9E+00	3.5E+03	3.5E+03	0.0E+00	2.8E+00	1.1E+02	2.8E+00	6.3E+01
214	1.4E+00	4.0E+00	6.5E+02	0.0E+00	2.8E-01	1.7E+00	2.0E+01	2.5E+02	2.0E+01	2.8E-01
215	5.4E+01	1.4E+02	1.8E+03	3.2E+00	5.1E-01	0.0E+00	1.3E+01	3.1E+03	1.3E+01	1.9E+00
216	1.2E+01	2.5E+02	8.2E+03	0.0E+00	0.0E+00	3.0E-01	5.1E+02	2.7E+03	5.1E+02	5.3E+02
217	2.5E+00	8.1E+00	1.8E+03	0.0E+00	1.5E+00	2.3E-01	1.9E+01	5.6E+02	1.9E+01	2.5E+01
218	6.8E+00	1.4E+02	4.7E+03	0.0E+00	0.0E+00	1.7E-01	2.9E+02	1.5E+03	2.9E+02	3.0E+02
219	0.0E+00	6.5E+02	1.7E+04	0.0E+00	6.8E+00	6.2E+00	2.7E+02	5.9E+03	2.7E+02	3.3E+02
220	0.0E+00	2.5E+02	6.6E+03	0.0E+00	2.6E+00	2.3E+00	1.0E+02	2.2E+03	1.0E+02	1.2E+02
221	1.7E+02	0.0E+00	2.0E+03	6.5E+01	8.6E+00	0.0E+00	1.2E+00	9.5E+02	1.2E+00	3.6E+02
222	0.0E+00	8.6E+02	1.7E+02	0.0E+00	0.0E+00	0.0E+00	7.1E+00	7.2E+02	7.1E+00	1.6E+03
223	9.5E+01	1.0E+03	1.3E+04	2.9E+02	2.1E-01	0.0E+00	2.0E+01	1.4E+04	2.0E+01	1.3E+02
224	7.8E+02	6.9E+00	2.0E+04	6.1E+00	4.1E+01	3.8E+00	9.4E+01	8.9E+03	9.4E+01	1.6E+03
225	1.2E+01	1.2E+02	1.6E+03	3.5E+01	2.5E-02	0.0E+00	2.4E+00	1.7E+03	2.4E+00	1.6E+01
226	0.0E+00	1.5E+01	2.6E+03	2.4E-01	1.1E+00	2.5E+00	1.6E+01	1.0E+03	1.6E+01	8.4E-01

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
227	0.0E+00	6.3E+01	1.1E+04	1.0E+00	4.5E+00	1.1E+01	6.6E+01	4.4E+03	6.6E+01	3.5E+00
228	0.0E+00	2.7E+01	2.2E+01	4.9E+01	6.1E+01	0.0E+00	2.8E+01	7.6E+01	2.8E+01	2.0E+02
229	0.0E+00	6.5E+02	2.7E+03	0.0E+00	0.0E+00	0.0E+00	2.3E+00	3.0E+03	2.3E+00	1.3E+03
230	2.2E+01	4.2E+01	1.4E+01	4.0E+03	6.0E+02	0.0E+00	7.4E+00	1.6E+02	7.4E+00	1.9E+01
231	1.0E+01	1.9E+01	6.4E+00	1.8E+03	2.7E+02	0.0E+00	3.4E+00	7.5E+01	3.4E+00	8.8E+00
232	9.7E+02	0.0E+00	1.1E+04	3.7E+02	4.8E+01	0.0E+00	6.7E+00	5.3E+03	6.7E+00	2.0E+03
233	2.4E+00	6.1E+00	1.4E+02	1.6E+02	4.2E+02	0.0E+00	9.1E+02	1.7E+03	9.1E+02	4.1E+01
234	5.9E+00	0.0E+00	0.0E+00	7.3E+02	4.5E+01	0.0E+00	0.0E+00	6.7E+00	0.0E+00	0.0E+00
235	3.9E+01	5.6E+00	6.4E+02	6.3E+00	1.6E+01	4.6E+00	7.2E+01	1.5E+02	7.2E+01	3.3E+01
236	6.7E+01	5.9E-01	1.7E+03	5.2E-01	3.5E+00	3.3E-01	8.0E+00	7.6E+02	8.0E+00	1.4E+02
237	1.7E+02	4.1E+02	4.5E+03	1.7E+00	0.0E+00	0.0E+00	1.7E+02	6.2E+03	1.7E+02	4.0E+00
238	7.0E+00	1.2E+01	7.6E+00	5.1E+01	5.8E-01	2.4E-01	2.6E+00	3.1E+01	2.6E+00	2.9E+00
239	0.0E+00	5.2E+02	1.4E+04	0.0E+00	5.4E+00	4.9E+00	2.2E+02	4.6E+03	2.2E+02	2.6E+02
240	6.9E+00	3.9E+01	7.8E+03	0.0E+00	3.1E+00	1.7E+01	1.3E+02	1.9E+04	1.3E+02	1.4E+03
241	9.1E+01	0.0E+00	1.0E+03	3.5E+01	4.5E+00	0.0E+00	6.3E-01	5.0E+02	6.3E-01	1.9E+02
242	3.0E-02	1.7E-01	3.3E+01	0.0E+00	1.3E-02	7.4E-02	5.4E-01	8.1E+01	5.4E-01	5.9E+00
243	2.7E+01	3.8E+00	4.4E+02	4.3E+00	1.1E+01	3.1E+00	4.9E+01	1.0E+02	4.9E+01	2.2E+01
244	2.5E+00	1.8E+03	9.7E+03	0.0E+00	0.0E+00	5.5E+00	2.4E+03	1.4E+04	2.4E+03	7.7E+03
245	5.4E+00	2.1E+01	5.1E+02	0.0E+00	0.0E+00	0.0E+00	1.1E+02	5.5E+02	1.1E+02	0.0E+00
246	1.6E+01	3.0E+01	1.0E+01	2.8E+03	4.3E+02	0.0E+00	5.3E+00	1.2E+02	5.3E+00	1.4E+01
247	5.2E+01	5.6E+02	7.3E+03	1.6E+02	1.1E-01	0.0E+00	1.1E+01	7.4E+03	1.1E+01	7.0E+01
248	1.2E+03	2.8E+03	3.1E+04	1.1E+01	0.0E+00	0.0E+00	1.1E+03	4.3E+04	1.1E+03	2.8E+01
249	0.0E+00	4.7E+02	9.3E+01	0.0E+00	0.0E+00	0.0E+00	3.9E+00	4.0E+02	3.9E+00	8.5E+02
250	8.9E+00	1.7E+01	5.6E+00	1.6E+03	2.4E+02	0.0E+00	3.0E+00	6.6E+01	3.0E+00	7.7E+00
251	1.4E+00	0.0E+00	1.4E+02	0.0E+00	9.6E-03	1.9E-02	5.7E-02	5.3E+01	5.7E-02	1.6E+01
252	0.0E+00	5.5E+02	2.2E+03	0.0E+00	0.0E+00	0.0E+00	1.9E+00	2.5E+03	1.9E+00	1.1E+03
253	3.9E+01	6.5E+01	4.2E+01	2.9E+02	3.2E+00	1.3E+00	1.4E+01	1.7E+02	1.4E+01	1.6E+01
254	1.9E+01	9.9E+00	1.9E+03	0.0E+00	0.0E+00	0.0E+00	2.0E+01	5.7E+02	2.0E+01	0.0E+00
255	4.8E+02	1.7E+02	1.1E+04	0.0E+00	0.0E+00	1.3E+01	8.0E+01	5.3E+03	8.0E+01	4.2E+00
256	7.3E+01	7.7E+02	1.0E+04	2.2E+02	1.6E-01	0.0E+00	1.5E+01	1.0E+04	1.5E+01	9.7E+01
257	4.6E+01	4.9E+02	6.4E+03	1.4E+02	1.0E-01	0.0E+00	9.5E+00	6.5E+03	9.5E+00	6.1E+01
258	3.0E+00	0.0E+00	3.0E+02	0.0E+00	2.1E-02	4.1E-02	1.2E-01	1.1E+02	1.2E-01	3.3E+01
259	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
260	3.8E+00	2.0E+00	3.9E+02	0.0E+00	0.0E+00	0.0E+00	4.0E+00	1.2E+02	4.0E+00	0.0E+00
261	0.0E+00	7.2E-02	3.4E+01	0.0E+00	3.8E-03	3.8E-03	7.2E-01	1.3E+01	7.2E-01	6.1E+00
262	0.0E+00	9.4E+00	1.6E+03	1.5E-01	6.8E-01	1.6E+00	9.8E+00	6.5E+02	9.8E+00	5.3E-01
263	3.0E+01	7.5E+01	9.6E+02	1.8E+00	2.8E-01	0.0E+00	7.1E+00	1.7E+03	7.1E+00	1.1E+00
264	2.0E+02	1.4E+02	9.8E+03	0.0E+00	0.0E+00	0.0E+00	6.9E+01	1.6E+04	6.9E+01	1.0E+02
265	1.4E+01	1.0E+01	6.9E+02	0.0E+00	0.0E+00	0.0E+00	4.9E+00	1.1E+03	4.9E+00	7.4E+00
266	5.3E+01	3.7E+01	2.6E+03	0.0E+00	0.0E+00	0.0E+00	1.8E+01	4.1E+03	1.8E+01	2.7E+01
267	6.8E+01	3.5E-01	2.0E+02	1.8E+01	1.3E+01	5.3E+00	4.3E+00	9.5E+01	4.3E+00	9.0E+01
268	2.6E+01	5.5E+02	1.8E+04	0.0E+00	0.0E+00	6.6E-01	1.1E+03	5.8E+03	1.1E+03	1.2E+03
269	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
270	1.6E+03	3.3E+03	5.9E+03	0.0E+00	0.0E+00	0.0E+00	3.3E+03	9.7E+03	3.3E+03	7.0E+02
271	3.0E+00	2.2E+03	1.2E+04	0.0E+00	0.0E+00	6.7E+00	2.9E+03	1.8E+04	2.9E+03	9.5E+03
272	2.7E+03	2.3E+03	1.2E+04	0.0E+00	0.0E+00	0.0E+00	1.5E+03	9.7E+03	1.5E+03	2.1E+02
273	3.9E+01	4.9E+01	2.0E+02	0.0E+00	0.0E+00	0.0E+00	1.5E+01	1.9E+02	1.5E+01	9.2E+01
274	1.1E+01	2.0E+01	6.7E+00	1.9E+03	2.8E+02	0.0E+00	3.5E+00	7.8E+01	3.5E+00	9.1E+00
275	9.2E+02	1.1E+03	4.6E+03	0.0E+00	0.0E+00	0.0E+00	3.5E+02	4.6E+03	3.5E+02	2.2E+03
276	1.0E+03	8.8E+00	2.5E+04	7.8E+00	5.2E+01	4.9E+00	1.2E+02	1.1E+04	1.2E+02	2.1E+03
277	7.1E+01	0.0E+00	7.1E+03	0.0E+00	4.9E-01	9.8E-01	2.9E+00	2.7E+03	2.9E+00	8.0E+02

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
278	0.0E+00	2.9E+02	8.5E+03	0.0E+00	0.0E+00	2.7E+00	1.4E+03	8.2E+03	1.4E+03	2.5E+02
279	1.4E+02	1.3E+00	3.6E+03	1.1E+00	7.4E+00	7.0E-01	1.7E+01	1.6E+03	1.7E+01	2.9E+02
280	0.0E+00	7.7E+02	2.2E+04	0.0E+00	0.0E+00	7.0E+00	3.7E+03	2.2E+04	3.7E+03	6.6E+02
281	8.5E-02	4.7E-01	4.6E+02	0.0E+00	4.8E-02	7.1E-03	1.2E+00	5.4E+01	1.2E+00	1.6E-01
282	1.4E+00	7.6E+00	7.4E+03	0.0E+00	7.7E-01	1.1E-01	1.9E+01	8.6E+02	1.9E+01	2.6E+00
283	0.0E+00	2.2E+01	5.2E+03	7.0E+00	0.0E+00	0.0E+00	4.8E+02	1.7E+03	4.8E+02	4.4E+00
284	0.0E+00	7.2E+01	1.7E+04	2.3E+01	0.0E+00	0.0E+00	1.5E+03	5.4E+03	1.5E+03	1.4E+01
285	7.2E+00	3.0E+02	1.8E+03	0.0E+00	4.4E-01	0.0E+00	0.0E+00	2.3E+03	0.0E+00	2.4E+02
286	6.2E+00	3.4E+01	3.3E+04	0.0E+00	3.5E+00	5.1E-01	8.3E+01	3.9E+03	8.3E+01	1.2E+01
287	9.0E+01	9.5E+01	1.1E+04	0.0E+00	1.3E+00	0.0E+00	4.4E+02	6.5E+03	4.4E+02	3.2E+01
288	4.9E+00	1.1E+01	6.5E+01	0.0E+00	1.2E+00	1.2E-01	2.8E-01	5.4E+02	2.8E-01	1.0E+02
289	0.0E+00	1.9E+01	1.2E+04	0.0E+00	0.0E+00	0.0E+00	2.8E+02	5.1E+03	2.8E+02	3.2E+01
290	1.2E+01	4.0E-01	8.8E+02	0.0E+00	4.7E+00	1.5E+02	4.0E-01	4.2E+03	4.0E-01	5.3E+02
291	3.6E+00	2.0E+01	1.0E+03	2.9E-01	0.0E+00	0.0E+00	7.7E+00	7.4E+02	7.7E+00	1.0E+02
292	1.1E+00	6.5E+00	3.3E+02	9.1E-02	0.0E+00	0.0E+00	2.5E+00	2.4E+02	2.5E+00	3.2E+01
293	1.3E+00	7.5E+00	3.8E+02	1.1E-01	0.0E+00	0.0E+00	2.8E+00	2.7E+02	2.8E+00	3.7E+01
294	4.0E+00	2.9E+00	2.0E+02	0.0E+00	0.0E+00	0.0E+00	1.4E+00	3.1E+02	1.4E+00	2.1E+00
295	2.4E+00	1.7E+00	1.2E+02	0.0E+00	0.0E+00	0.0E+00	8.2E-01	1.9E+02	8.2E-01	1.2E+00
296	9.5E-01	6.7E-01	4.7E+01	0.0E+00	0.0E+00	0.0E+00	3.3E-01	7.4E+01	3.3E-01	4.9E-01
297	0.0E+00	3.8E+00	2.4E+03	0.0E+00	0.0E+00	0.0E+00	5.5E+01	1.0E+03	5.5E+01	6.3E+00
298	2.0E+00	1.2E+01	5.9E+02	1.6E-01	0.0E+00	0.0E+00	4.4E+00	4.2E+02	4.4E+00	5.7E+01
299	6.4E+00	1.2E+01	4.0E+00	1.1E+03	1.7E+02	0.0E+00	2.1E+00	4.7E+01	2.1E+00	5.5E+00
300	1.3E+02	4.6E+01	3.1E+03	0.0E+00	0.0E+00	3.4E+00	2.2E+01	1.4E+03	2.2E+01	1.1E+00
301	3.6E+02	3.2E+00	9.1E+03	2.8E+00	1.9E+01	1.8E+00	4.3E+01	4.1E+03	4.3E+01	7.4E+02
302	4.2E+02	1.5E+02	1.0E+04	0.0E+00	0.0E+00	1.1E+01	7.0E+01	4.6E+03	7.0E+01	3.6E+00
303	3.9E+00	7.3E+00	2.4E+00	6.9E+02	1.0E+02	0.0E+00	1.3E+00	2.8E+01	1.3E+00	3.3E+00
304	1.0E+02	4.0E+02	9.6E+03	0.0E+00	0.0E+00	0.0E+00	2.0E+03	1.0E+04	2.0E+03	0.0E+00
305	7.0E+00	3.2E+01	4.0E+00	3.4E+03	3.7E+02	0.0E+00	9.0E+01	5.3E+02	9.0E+01	7.0E+01
306	3.5E+03	2.4E+03	2.8E+04	0.0E+00	0.0E+00	0.0E+00	1.4E+03	1.5E+04	1.4E+03	1.9E+02
307	0.0E+00	1.4E+01	1.1E+01	2.6E+01	3.2E+01	0.0E+00	1.5E+01	3.9E+01	1.5E+01	1.0E+02
308	7.6E+00	0.0E+00	9.0E+03	0.0E+00	7.4E+01	5.6E-01	2.8E+02	2.6E+03	2.8E+02	2.2E+01
309	3.1E+03	2.2E+03	2.5E+04	0.0E+00	0.0E+00	0.0E+00	1.3E+03	1.3E+04	1.3E+03	1.7E+02
310	0.0E+00	2.5E+01	4.3E+03	4.0E-01	1.8E+00	4.2E+00	2.6E+01	1.7E+03	2.6E+01	1.4E+00
311	4.2E+01	8.8E+02	2.9E+04	0.0E+00	0.0E+00	1.1E+00	1.8E+03	9.4E+03	1.8E+03	1.9E+03
312	1.2E+01	0.0E+00	1.3E+03	0.0E+00	8.6E-02	1.7E-01	5.2E-01	4.8E+02	5.2E-01	1.4E+02
313	1.1E+01	5.0E+01	6.2E+00	5.2E+03	5.7E+02	0.0E+00	1.4E+02	8.2E+02	1.4E+02	1.1E+02
314	6.6E+03	4.6E+03	5.4E+04	0.0E+00	0.0E+00	0.0E+00	2.7E+03	2.9E+04	2.7E+03	3.6E+02
315	1.1E+02	1.1E+03	1.5E+04	3.2E+02	2.3E-01	0.0E+00	2.2E+01	1.5E+04	2.2E+01	1.4E+02
316	4.7E+01	1.8E+02	4.4E+03	0.0E+00	0.0E+00	0.0E+00	9.4E+02	4.8E+03	9.4E+02	0.0E+00
317	6.3E+02	1.3E+03	2.3E+03	0.0E+00	0.0E+00	0.0E+00	1.3E+03	3.8E+03	1.3E+03	2.7E+02
318	3.7E+00	7.0E+00	2.4E+00	6.6E+02	1.0E+02	0.0E+00	1.2E+00	2.7E+01	1.2E+00	3.2E+00
319	1.8E+01	3.3E+01	1.1E+01	3.1E+03	4.7E+02	0.0E+00	5.9E+00	1.3E+02	5.9E+00	1.5E+01
320	2.6E+01	5.5E+02	1.8E+04	0.0E+00	0.0E+00	6.6E-01	1.1E+03	5.8E+03	1.1E+03	1.2E+03
321	1.4E+01	2.6E+01	8.7E+00	2.5E+03	3.7E+02	0.0E+00	4.6E+00	1.0E+02	4.6E+00	1.2E+01
322	1.4E+01	2.7E+01	9.1E+00	2.6E+03	3.8E+02	0.0E+00	4.8E+00	1.1E+02	4.8E+00	1.2E+01
323	0.0E+00	5.6E+02	1.1E+02	0.0E+00	0.0E+00	0.0E+00	4.6E+00	4.7E+02	4.6E+00	1.0E+03
324	1.2E+00	2.1E+00	1.4E+00	9.2E+00	1.0E-01	4.3E-02	4.6E-01	5.5E+00	4.6E-01	5.2E-01
325	2.8E+02	2.4E+00	7.0E+03	2.2E+00	1.5E+01	1.4E+00	3.3E+01	3.2E+03	3.3E+01	5.7E+02
326	8.0E+00	1.5E+01	5.0E+00	1.4E+03	2.1E+02	0.0E+00	2.7E+00	5.8E+01	2.7E+00	6.9E+00
327	0.0E+00	2.8E+02	5.6E+01	0.0E+00	0.0E+00	0.0E+00	2.3E+00	2.4E+02	2.3E+00	5.1E+02
328	1.0E+00	8.8E-03	2.5E+01	7.9E-03	5.2E-02	4.9E-03	1.2E-01	1.1E+01	1.2E-01	2.1E+00

Table D.10: .-Available rainfed area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn F	Corn	Sorgo	Oat	Wheat	Rye	Barley F
329	2.3E+01	1.2E+01	2.3E+03	0.0E+00	0.0E+00	0.0E+00	2.4E+01	7.1E+02	2.4E+01	0.0E+00
330	3.5E-01	1.2E+00	2.5E+02	0.0E+00	2.2E-01	3.3E-02	2.7E+00	8.1E+01	2.7E+00	3.6E+00
331	3.3E-03	2.7E+00	2.6E+01	0.0E+00	0.0E+00	0.0E+00	6.8E+00	1.7E+01	6.8E+00	2.7E+00
332	5.5E-02	4.5E+01	4.4E+02	0.0E+00	0.0E+00	0.0E+00	1.2E+02	2.8E+02	1.2E+02	4.6E+01
333	1.2E+02	3.1E+02	4.0E+03	7.2E+00	1.2E+00	0.0E+00	2.9E+01	7.0E+03	2.9E+01	4.3E+00
334	9.9E+00	5.3E+00	1.0E+03	0.0E+00	0.0E+00	0.0E+00	1.0E+01	3.1E+02	1.0E+01	0.0E+00
335	1.2E+02	0.0E+00	1.4E+03	4.7E+01	6.2E+00	0.0E+00	8.6E-01	6.9E+02	8.6E-01	2.6E+02
336	1.9E+02	0.0E+00	2.2E+03	7.3E+01	9.6E+00	0.0E+00	1.3E+00	1.1E+03	1.3E+00	4.0E+02
337	3.6E+00	0.0E+00	0.0E+00	4.5E+02	2.7E+01	0.0E+00	0.0E+00	4.1E+00	0.0E+00	0.0E+00
338	9.9E+00	0.0E+00	1.2E+04	0.0E+00	9.6E+01	7.2E-01	3.6E+02	3.3E+03	3.6E+02	2.9E+01
339	2.5E-01	1.0E+01	6.1E+01	0.0E+00	1.5E-02	0.0E+00	0.0E+00	7.8E+01	0.0E+00	8.4E+00
340	7.5E+00	1.9E+01	4.3E+02	5.0E+02	1.3E+03	0.0E+00	2.8E+03	5.2E+03	2.8E+03	1.3E+02
341	3.8E+00	7.1E+00	2.4E+00	6.7E+02	1.0E+02	0.0E+00	1.3E+00	2.8E+01	1.3E+00	3.2E+00
342	3.1E+00	8.8E+00	1.4E+03	0.0E+00	6.3E-01	3.8E+00	4.3E+01	5.6E+02	4.3E+01	6.3E-01
343	4.4E-01	3.2E+02	1.7E+03	0.0E+00	0.0E+00	9.7E-01	4.2E+02	2.5E+03	4.2E+02	1.4E+03
344	5.8E+01	2.5E+01	0.0E+00	1.3E+02	6.7E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.6E+01
345	6.2E+02	6.5E+01	5.4E+04	0.0E+00	2.1E+01	4.1E+00	1.2E+03	3.3E+04	1.2E+03	1.8E+01

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
1	2.7E+02	3.3E+01	3.1E+02	7.0E+01	8.7E+00	9.3E-02	3.3E+01	7.1E+01	1.9E+01	1.3E+01
2	1.3E+02	2.2E+01	7.0E+02	3.0E+01	6.0E+02	3.9E+00	1.8E+02	9.7E+01	0.0E+00	1.6E+01
3	8.8E+00	0.0E+00	6.9E+00	1.5E+00	9.2E+00	0.0E+00	0.0E+00	4.9E-01	0.0E+00	0.0E+00
4	4.2E+01	6.9E+00	9.6E+02	0.0E+00	2.7E+00	3.8E+00	5.6E+01	9.1E+01	2.1E+00	3.0E-01
5	4.1E+01	0.0E+00	8.6E+02	0.0E+00	9.2E+01	7.9E+00	4.1E+01	6.1E+01	9.9E-01	1.2E+00
6	3.0E+00	0.0E+00	6.4E+01	0.0E+00	1.3E+00	5.9E-01	3.1E+00	4.2E+00	7.4E-02	9.2E-02
7	1.1E+02	5.0E+00	2.0E+02	4.2E+00	7.6E+00	1.5E+00	1.5E+02	3.9E+00	1.6E+00	1.8E+01
8	2.8E+01	3.9E+00	5.7E+01	7.3E+00	9.1E+00	0.0E+00	9.1E+00	5.2E+00	2.4E+00	0.0E+00
9	1.8E+02	2.9E+00	5.6E+02	1.8E+01	8.4E+01	1.1E+00	1.3E+02	8.7E+00	6.6E+00	1.8E+01
10	6.2E+01	4.2E+01	1.5E+03	0.0E+00	4.8E+01	1.5E+01	3.0E+01	1.4E+03	8.6E+01	0.0E+00
11	1.2E+01	0.0E+00	9.6E+00	2.1E+00	1.5E+02	0.0E+00	0.0E+00	1.5E+01	0.0E+00	0.0E+00
12	1.2E+00	2.3E-02	4.3E+00	9.1E-02	7.9E-02	2.3E-02	2.1E+00	1.2E+00	3.4E-02	5.0E-01
13	1.0E+03	1.2E+01	1.5E+03	1.0E+03	1.7E+03	8.8E+01	7.5E+01	1.1E+03	7.0E+01	6.4E+02
14	1.4E+00	2.7E-02	5.1E+00	1.1E-01	9.5E-02	2.7E-02	2.5E+00	1.4E+00	4.1E-02	6.0E-01
15	2.2E+00	2.8E-01	2.0E+00	1.9E-01	9.2E-01	9.4E-02	7.3E-01	3.3E-01	2.4E-02	5.4E-01
16	1.2E+00	4.8E-02	4.5E+00	7.0E-01	1.0E+00	0.0E+00	9.1E-01	1.0E+00	0.0E+00	0.0E+00
17	2.8E+02	0.0E+00	4.0E+02	6.9E+01	5.1E+02	7.8E+00	9.6E+00	1.5E+02	1.4E+00	4.7E+01
18	3.8E+00	4.5E+00	1.3E+01	5.7E+00	1.4E+01	0.0E+00	1.5E+01	7.4E+01	0.0E+00	1.1E+01
19	3.9E-01	4.6E-01	1.3E+00	5.9E-01	1.5E+00	0.0E+00	1.6E+00	7.6E+00	0.0E+00	1.2E+00
20	1.2E+01	0.0E+00	4.9E+01	1.3E+01	1.4E+00	0.0E+00	5.9E+00	2.0E+01	0.0E+00	1.7E+01
21	1.4E+02	9.0E+01	6.7E+02	0.0E+00	9.1E+01	1.4E+00	4.7E+02	9.8E+02	0.0E+00	5.9E+01
22	2.2E-01	0.0E+00	0.0E+00	6.8E+00	4.2E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
23	8.2E+00	5.6E+00	2.0E+02	0.0E+00	6.4E+00	2.1E+00	4.0E+00	1.9E+02	1.1E+01	0.0E+00
24	1.9E+02	0.0E+00	5.0E+02	2.7E+01	4.2E+02	3.2E+00	3.3E+01	2.0E+02	2.5E+00	6.3E-01
25	7.4E+02	2.1E+02	3.7E+03	4.0E+02	3.5E+02	0.0E+00	4.3E+01	2.4E+03	0.0E+00	1.6E+02
26	1.1E+02	2.1E+01	4.4E+02	6.0E+01	5.4E+01	0.0E+00	1.8E+01	5.1E+02	2.1E+01	0.0E+00
27	1.6E+02	2.8E+01	6.2E+02	8.3E+01	7.5E+01	0.0E+00	2.5E+01	7.1E+02	3.0E+01	0.0E+00

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
28	5.4E-01	0.0E+00	0.0E+00	1.7E+01	1.0E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
29	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
30	3.9E+02	1.4E+02	3.0E+02	1.6E+02	3.8E+03	5.6E-01	1.3E+02	1.2E+03	6.9E+01	7.5E+00
31	1.9E+01	5.3E+00	9.5E+01	1.0E+01	9.0E+00	0.0E+00	1.1E+00	6.1E+01	0.0E+00	4.2E+00
32	3.8E+00	0.0E+00	3.0E+00	6.5E-01	4.7E+01	0.0E+00	0.0E+00	4.6E+00	0.0E+00	0.0E+00
33	5.5E+02	0.0E+00	4.3E+02	9.2E+01	6.8E+03	0.0E+00	0.0E+00	6.5E+02	0.0E+00	0.0E+00
34	2.9E+01	0.0E+00	1.2E+02	3.2E+01	3.4E+00	0.0E+00	1.4E+01	4.9E+01	0.0E+00	4.0E+01
35	1.9E+01	3.7E-01	6.9E+01	1.5E+00	1.3E+00	3.7E-01	3.4E+01	2.0E+01	5.5E-01	8.1E+00
36	8.9E+02	1.1E+01	1.3E+03	9.0E+02	1.5E+03	7.7E+01	6.6E+01	9.3E+02	6.1E+01	5.6E+02
37	1.3E+02	1.4E+01	3.7E+03	0.0E+00	6.9E+02	7.6E+01	2.9E+02	8.9E+02	1.5E+02	6.3E+00
38	4.3E+03	1.0E+02	9.0E+03	0.0E+00	1.1E+04	5.6E+01	1.1E+02	2.4E+03	9.0E+00	2.7E+00
39	4.7E+01	0.0E+00	4.4E+02	5.1E+00	7.0E+01	4.6E+01	8.5E+01	9.5E+01	0.0E+00	1.4E+02
40	5.4E+01	0.0E+00	2.2E+02	6.0E+01	6.2E+00	0.0E+00	2.6E+01	9.0E+01	0.0E+00	7.4E+01
41	4.6E+00	5.9E-01	4.1E+00	3.9E-01	1.9E+00	2.0E-01	1.5E+00	6.9E-01	4.9E-02	1.1E+00
42	8.2E-01	0.0E+00	7.6E+00	8.8E-02	1.2E+00	7.9E-01	1.5E+00	1.6E+00	0.0E+00	2.4E+00
43	2.0E+01	5.7E+00	1.0E+02	1.1E+01	9.7E+00	0.0E+00	1.2E+00	6.5E+01	0.0E+00	4.5E+00
44	2.5E+02	1.2E+01	4.6E+02	9.9E+00	2.1E+02	3.5E+00	3.5E+02	1.5E+02	3.7E+00	4.2E+01
45	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
46	1.7E+03	2.3E+02	3.4E+03	4.3E+02	4.7E+03	0.0E+00	5.4E+02	2.7E+03	1.4E+02	0.0E+00
47	3.6E+00	0.0E+00	1.5E+01	4.0E+00	4.1E-01	0.0E+00	1.8E+00	6.0E+00	0.0E+00	4.9E+00
48	6.0E+01	2.2E+01	4.6E+01	2.5E+01	6.0E+02	8.6E-02	2.1E+01	1.9E+02	1.1E+01	1.2E+00
49	6.2E+02	7.7E+01	7.3E+02	1.6E+02	1.8E+02	2.2E-01	7.7E+01	1.1E+03	4.5E+01	3.0E+01
50	2.9E-01	0.0E+00	0.0E+00	8.9E+00	5.5E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
51	2.9E+03	9.1E+00	3.0E+03	0.0E+00	1.2E+03	2.3E+01	3.7E+01	2.4E+03	7.9E+00	2.4E-01
52	9.4E-01	0.0E+00	2.9E-01	4.3E-01	5.0E+01	7.4E-02	0.0E+00	9.1E-01	0.0E+00	0.0E+00
53	1.4E+02	2.5E+01	5.4E+02	7.3E+01	6.6E+01	0.0E+00	2.2E+01	6.2E+02	2.6E+01	0.0E+00
54	5.4E+01	3.7E+01	1.3E+03	0.0E+00	4.2E+01	1.4E+01	2.6E+01	1.3E+03	7.5E+01	0.0E+00
55	3.7E+00	0.0E+00	1.2E+00	1.7E+00	2.0E+02	2.9E-01	0.0E+00	3.6E+00	0.0E+00	0.0E+00
56	7.9E+02	2.5E+00	8.1E+02	0.0E+00	3.4E+02	6.1E+00	1.0E+01	6.4E+02	2.1E+00	6.4E-02
57	1.6E+02	0.0E+00	4.3E+02	2.3E+01	3.6E+02	2.7E+00	2.9E+01	1.7E+02	2.2E+00	5.4E-01
58	9.6E+01	0.0E+00	2.0E+03	0.0E+00	1.6E+03	1.9E+01	9.7E+01	1.1E+03	2.3E+00	2.9E+00
59	9.9E+01	0.0E+00	1.7E+02	0.0E+00	2.3E+02	5.3E+00	1.1E+02	9.2E+02	9.1E-02	2.3E+01
60	7.1E+02	0.0E+00	1.2E+03	0.0E+00	1.7E+03	3.8E+01	8.2E+02	6.6E+03	6.6E-01	1.6E+02
61	1.0E+03	0.0E+00	5.2E+02	1.8E+02	1.4E+03	7.2E+02	4.8E+02	3.4E+03	0.0E+00	4.2E+02
62	2.1E+02	1.2E+01	2.8E+02	5.7E+01	1.9E+02	3.7E+00	2.1E+02	5.3E+02	0.0E+00	8.6E+01
63	3.9E+01	2.2E+00	5.4E+01	1.1E+01	3.7E+01	7.0E-01	4.1E+01	1.0E+02	0.0E+00	1.6E+01
64	5.6E+01	1.1E+00	2.0E+02	4.3E+00	3.8E+00	1.1E+00	1.0E+02	5.7E+01	1.6E+00	2.4E+01
65	2.8E+02	2.3E+02	8.1E+03	8.6E+00	7.2E+02	2.6E+01	9.4E+02	1.2E+03	3.2E+01	0.0E+00
66	1.4E+02	8.7E+00	4.9E+02	2.8E+01	3.9E+01	1.6E+00	5.0E+02	2.4E+02	0.0E+00	5.2E+00
67	8.8E+01	0.0E+00	4.5E+01	1.6E+01	1.2E+02	6.2E+01	4.1E+01	2.9E+02	0.0E+00	3.6E+01
68	5.0E+01	4.2E+01	1.5E+03	1.6E+00	1.3E+02	4.6E+00	1.7E+02	2.2E+02	5.7E+00	0.0E+00
69	4.8E+00	0.0E+00	4.5E+01	5.2E-01	7.2E+00	4.7E+00	8.6E+00	9.7E+00	0.0E+00	1.4E+01
70	2.0E+01	4.0E-01	7.4E+01	1.6E+00	1.4E+00	4.0E-01	3.7E+01	2.1E+01	5.9E-01	8.7E+00
71	2.2E+00	4.2E-02	8.0E+00	1.7E-01	1.5E-01	4.2E-02	3.9E+00	2.2E+00	6.3E-02	9.3E-01
72	6.8E+03	8.5E+02	8.1E+03	1.8E+03	2.0E+03	2.4E+00	8.4E+02	1.2E+04	4.9E+02	3.3E+02
73	4.0E+01	2.7E+01	9.7E+02	0.0E+00	3.1E+01	9.9E+00	1.9E+01	9.1E+02	5.5E+01	0.0E+00
74	1.3E+01	5.3E-01	5.0E+01	7.7E+00	1.2E+01	0.0E+00	1.0E+01	1.1E+01	0.0E+00	0.0E+00
75	1.1E+03	1.5E+02	2.2E+03	2.8E+02	3.1E+03	0.0E+00	3.5E+02	1.8E+03	9.5E+01	0.0E+00
76	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
77	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
78	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
79	6.0E-02	0.0E+00	0.0E+00	1.9E+00	1.2E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
80	1.8E+03	5.7E+00	1.9E+03	0.0E+00	7.7E+02	1.4E+01	2.3E+01	1.5E+03	4.9E+00	1.5E-01
81	9.7E+00	0.0E+00	7.6E+00	1.6E+00	1.2E+02	0.0E+00	0.0E+00	1.2E+01	0.0E+00	0.0E+00
82	6.8E+00	0.0E+00	0.0E+00	1.1E+02	1.6E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
83	3.9E+01	1.4E-01	1.8E+01	1.9E+00	4.6E+00	4.1E-01	2.8E+01	1.6E+01	1.0E-01	9.2E-01
84	1.5E+03	0.0E+00	7.3E+03	1.4E+02	1.4E+03	0.0E+00	0.0E+00	4.2E+03	0.0E+00	0.0E+00
85	3.4E+03	5.8E+01	1.1E+04	3.6E+02	3.6E+03	2.1E+01	2.5E+03	1.0E+04	1.3E+02	3.6E+02
86	1.8E+00	1.1E-01	6.4E+00	3.6E-01	5.0E-01	2.1E-02	6.6E+00	3.1E+00	0.0E+00	6.8E-02
87	4.6E-01	0.0E+00	0.0E+00	1.4E+01	8.8E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
88	9.1E+01	1.1E+00	1.3E+02	9.1E+01	1.5E+02	7.8E+00	6.6E+00	9.4E+01	6.2E+00	5.6E+01
89	2.5E+01	3.2E+00	3.0E+01	6.7E+00	7.5E+00	8.9E-03	3.1E+00	4.5E+01	1.8E+00	1.2E+00
90	1.9E+01	3.4E+00	1.1E+02	4.6E+00	4.0E+02	6.0E-01	2.8E+01	1.4E+02	0.0E+00	2.4E+00
91	5.2E+02	0.0E+00	7.4E+02	1.3E+02	9.5E+02	1.5E+01	1.8E+01	2.9E+02	2.7E+00	8.7E+01
92	2.4E-01	0.0E+00	2.2E+00	2.6E-02	3.5E-01	2.3E-01	4.3E-01	4.8E-01	0.0E+00	7.0E-01
93	1.6E+01	1.9E+01	5.3E+01	2.4E+01	6.0E+01	0.0E+00	6.3E+01	3.1E+02	0.0E+00	4.7E+01
94	2.4E+01	2.8E+01	8.0E+01	3.6E+01	9.0E+01	0.0E+00	9.5E+01	4.6E+02	0.0E+00	7.1E+01
95	9.1E+01	0.0E+00	2.8E+01	4.2E+01	4.8E+03	7.1E+00	0.0E+00	8.8E+01	0.0E+00	0.0E+00
96	8.6E-01	0.0E+00	0.0E+00	1.4E+01	2.1E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
97	1.1E+01	1.3E+01	3.8E+01	1.7E+01	4.3E+01	0.0E+00	4.5E+01	2.2E+02	0.0E+00	3.4E+01
98	1.4E+02	0.0E+00	7.1E+01	2.5E+01	1.9E+02	9.7E+01	6.5E+01	4.6E+02	0.0E+00	5.6E+01
99	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
100	4.8E+02	6.7E+01	4.6E+03	4.0E+02	6.6E+01	5.9E+01	1.1E+02	3.5E+03	3.1E+02	3.9E+02
101	1.6E+02	1.8E+01	4.7E+03	0.0E+00	9.0E+02	9.9E+01	3.7E+02	1.2E+03	2.0E+02	8.3E+00
102	3.7E+01	5.3E+00	8.9E+01	2.0E+01	1.0E+02	8.1E-02	4.4E+00	9.7E+01	2.7E-02	1.2E-01
103	2.1E-01	0.0E+00	0.0E+00	6.7E+00	4.1E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
104	3.1E+02	9.6E-01	3.2E+02	0.0E+00	1.3E+02	2.4E+00	3.9E+00	2.5E+02	8.3E-01	2.5E-02
105	4.0E+01	8.4E-01	4.6E+01	7.4E+00	1.1E+02	3.9E+00	2.6E+01	2.9E+02	0.0E+00	1.2E+01
106	4.1E+02	0.0E+00	2.1E+02	7.3E+01	5.6E+02	2.9E+02	1.9E+02	1.4E+03	0.0E+00	1.7E+02
107	8.1E+02	3.7E+01	1.5E+03	3.2E+01	6.6E+02	1.1E+01	1.1E+03	4.8E+02	1.2E+01	1.4E+02
108	1.7E+01	3.0E+00	6.5E+01	8.8E+00	8.0E+00	0.0E+00	2.6E+00	7.5E+01	3.2E+00	0.0E+00
109	1.1E+03	0.0E+00	8.9E+02	1.9E+02	1.4E+04	0.0E+00	0.0E+00	1.4E+03	0.0E+00	0.0E+00
110	2.2E+03	3.0E+02	4.4E+03	5.5E+02	6.0E+03	0.0E+00	6.9E+02	3.5E+03	1.9E+02	0.0E+00
111	1.7E+04	5.1E+01	1.7E+04	0.0E+00	7.0E+03	1.3E+02	2.1E+02	1.3E+04	4.4E+01	1.3E+00
112	2.6E+03	5.4E+01	4.4E+01	4.7E+02	1.1E+02	3.8E+00	2.5E+01	2.8E+02	0.0E+00	8.0E+02
113	1.5E+00	0.0E+00	0.0E+00	7.0E-01	3.9E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
114	2.1E+03	2.7E+02	2.5E+03	5.6E+02	6.3E+02	7.5E-01	2.6E+02	3.8E+03	1.5E+02	1.0E+02
115	2.5E+01	1.4E+00	3.4E+01	6.9E+00	2.3E+01	4.5E-01	2.6E+01	6.4E+01	0.0E+00	1.0E+01
116	2.9E+03	1.1E+03	2.2E+03	1.2E+03	2.9E+04	4.2E+00	1.0E+03	8.9E+03	5.1E+02	5.6E+01
117	2.1E+00	8.7E-02	8.3E+00	1.3E+00	1.9E+00	0.0E+00	1.7E+00	1.9E+00	0.0E+00	0.0E+00
118	1.9E+03	6.8E+02	1.4E+03	7.7E+02	1.9E+04	2.7E+00	6.4E+02	5.8E+03	3.3E+02	3.6E+01
119	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
120	3.3E-01	0.0E+00	0.0E+00	1.0E+01	6.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
121	1.1E+01	1.9E+00	5.9E+01	2.5E+00	2.2E+02	3.3E-01	1.5E+01	7.5E+01	0.0E+00	1.3E+00
122	1.1E+01	0.0E+00	9.7E-01	3.3E+01	4.7E+01	0.0E+00	1.4E+00	2.0E-01	0.0E+00	2.0E+00
123	1.7E+02	7.0E+00	6.6E+02	1.0E+02	1.5E+02	0.0E+00	1.3E+02	1.5E+02	0.0E+00	0.0E+00
124	6.3E+02	0.0E+00	9.1E+02	1.6E+02	1.2E+03	1.8E+01	2.2E+01	3.5E+02	3.3E+00	1.1E+02
125	1.5E+02	1.8E+00	2.2E+02	1.5E+02	2.5E+02	1.3E+01	1.1E+01	1.6E+02	1.0E+01	9.3E+01
126	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
127	4.3E+02	5.1E+00	6.4E+02	4.3E+02	7.1E+02	3.7E+01	3.2E+01	4.5E+02	3.0E+01	2.7E+02
128	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
129	1.5E+01	0.0E+00	1.3E+00	4.3E+01	6.2E+01	0.0E+00	1.8E+00	2.6E-01	0.0E+00	2.6E+00

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
130	1.8E+00	5.1E-01	9.2E+00	9.9E-01	8.7E-01	0.0E+00	1.1E-01	5.9E+00	0.0E+00	4.1E-01
131	6.3E+01	4.1E+01	3.1E+02	0.0E+00	4.2E+01	6.5E-01	2.2E+02	4.5E+02	0.0E+00	2.7E+01
132	4.5E+00	0.0E+00	1.2E+01	6.4E-01	1.0E+01	7.6E-02	8.1E-01	4.8E+00	6.1E-02	1.5E-02
133	4.6E+02	2.1E+01	8.3E+02	1.8E+01	3.7E+02	6.4E+00	6.3E+02	2.7E+02	6.8E+00	7.6E+01
134	1.1E+02	1.4E+01	1.3E+02	3.0E+01	3.3E+01	3.9E-02	1.4E+01	2.0E+02	8.1E+00	5.5E+00
135	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
136	5.6E+02	9.4E+00	1.8E+03	5.9E+01	5.9E+02	3.3E+00	4.1E+02	1.6E+03	2.1E+01	5.9E+01
137	3.3E+00	0.0E+00	2.5E+00	5.5E-01	4.0E+01	0.0E+00	0.0E+00	3.9E+00	0.0E+00	0.0E+00
138	4.2E+00	0.0E+00	1.3E+00	1.9E+00	2.2E+02	3.3E-01	0.0E+00	4.1E+00	0.0E+00	0.0E+00
139	2.6E+00	1.1E-01	9.9E+00	1.5E+00	2.3E+00	0.0E+00	2.0E+00	2.3E+00	0.0E+00	0.0E+00
140	7.8E+03	1.8E+02	1.6E+04	0.0E+00	1.9E+04	1.0E+02	2.1E+02	4.4E+03	1.6E+01	4.9E+00
141	3.5E+01	3.9E+00	1.0E+03	0.0E+00	1.9E+02	2.1E+01	7.9E+01	2.4E+02	4.2E+01	1.7E+00
142	4.8E+01	1.9E+00	1.8E+02	2.8E+01	4.2E+01	0.0E+00	3.7E+01	4.2E+01	0.0E+00	0.0E+00
143	3.3E+02	1.5E+01	5.9E+02	1.3E+01	2.7E+02	4.6E+00	4.5E+02	2.0E+02	4.9E+00	5.5E+01
144	6.7E+01	0.0E+00	0.0E+00	7.7E+00	1.0E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
145	0.0E+00	0.0E+00	0.0E+00	1.3E+00	5.2E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
146	1.3E-01	0.0E+00	0.0E+00	3.9E+00	2.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
147	5.7E-02	7.1E-03	2.4E-03	1.1E-01	3.3E-01	0.0E+00	2.4E-03	2.4E-02	0.0E+00	5.7E-02
148	1.1E+00	1.4E-01	4.6E-02	2.2E+00	6.5E+00	0.0E+00	4.6E-02	4.6E-01	0.0E+00	1.1E+00
149	3.7E+00	4.7E-01	1.6E-01	7.3E+00	2.2E+01	0.0E+00	1.6E-01	1.6E+00	0.0E+00	3.7E+00
150	9.3E+01	4.3E+00	1.7E+02	3.7E+00	7.6E+01	1.3E+00	1.3E+02	5.5E+01	1.4E+00	1.6E+01
151	1.8E+02	4.1E+00	3.6E+02	0.0E+00	4.3E+02	2.3E+00	4.6E+00	9.7E+01	3.6E-01	1.1E-01
152	2.6E+01	0.0E+00	8.0E+00	1.2E+01	1.4E+03	2.0E+00	0.0E+00	2.5E+01	0.0E+00	0.0E+00
153	2.0E+01	0.0E+00	1.6E+01	3.4E+00	2.5E+02	0.0E+00	0.0E+00	2.4E+01	0.0E+00	0.0E+00
154	1.6E+03	4.9E+00	1.6E+03	0.0E+00	6.6E+02	1.2E+01	2.0E+01	1.3E+03	4.2E+00	1.3E-01
155	7.3E+02	2.6E+02	5.6E+02	3.0E+02	7.2E+03	1.0E+00	2.5E+02	2.2E+03	1.3E+02	1.4E+01
156	2.3E+01	8.3E+00	1.8E+01	9.5E+00	2.3E+02	3.3E-02	7.9E+00	7.0E+01	4.0E+00	4.4E-01
157	9.2E+04	1.9E+03	1.5E+03	1.7E+04	3.7E+03	1.3E+02	8.5E+02	9.6E+03	0.0E+00	2.8E+04
158	2.3E+02	1.1E+01	4.2E+02	9.1E+00	1.9E+02	3.3E+00	3.2E+02	1.4E+02	3.5E+00	3.9E+01
159	3.7E+00	1.5E-01	1.4E+01	2.2E+00	3.3E+00	0.0E+00	2.9E+00	3.3E+00	0.0E+00	0.0E+00
160	1.9E+02	4.1E+01	4.6E+02	5.5E+01	1.8E+02	1.6E-01	1.2E+02	1.8E+02	8.9E+00	2.6E+01
161	6.9E+03	1.6E+02	1.4E+04	0.0E+00	1.7E+04	8.9E+01	1.8E+02	3.8E+03	1.4E+01	4.3E+00
162	8.8E+01	5.0E+00	1.2E+02	2.4E+01	8.2E+01	1.6E+00	9.1E+01	2.3E+02	0.0E+00	3.7E+01
163	1.1E+03	2.3E+02	2.6E+03	3.1E+02	1.0E+03	9.3E-01	6.8E+02	1.0E+03	5.1E+01	1.5E+02
164	3.1E+00	1.1E+00	2.4E+00	1.3E+00	3.0E+01	4.4E-03	1.1E+00	9.5E+00	5.4E-01	5.9E-02
165	2.2E+01	8.1E+00	1.7E+01	9.3E+00	2.2E+02	3.2E-02	7.8E+00	6.9E+01	4.0E+00	4.3E-01
166	2.9E+01	3.8E+00	2.6E+01	2.5E+00	1.2E+01	1.3E+00	9.7E+00	4.4E+00	3.1E-01	7.2E+00
167	6.1E+02	1.1E+02	2.4E+03	3.2E+02	2.9E+02	0.0E+00	9.5E+01	2.7E+03	1.1E+02	0.0E+00
168	3.7E+02	4.4E+00	5.5E+02	3.8E+02	6.2E+02	3.2E+01	2.8E+01	3.9E+02	2.6E+01	2.3E+02
169	5.2E+00	9.3E-01	2.9E+01	1.3E+00	1.1E+02	1.6E-01	7.5E+00	3.7E+01	0.0E+00	6.5E-01
170	1.3E+02	0.0E+00	2.3E+02	0.0E+00	3.1E+02	7.0E+00	1.5E+02	1.2E+03	1.2E-01	3.0E+01
171	8.8E+01	1.8E+00	4.9E+01	1.6E+01	1.2E+02	4.2E+00	2.8E+01	3.1E+02	0.0E+00	2.7E+01
172	8.9E+02	1.9E+01	1.6E+01	1.6E+02	4.0E+01	1.4E+00	9.2E+00	1.0E+02	0.0E+00	2.7E+02
173	1.3E+05	2.7E+03	8.0E+02	2.4E+04	2.0E+03	6.9E+01	4.5E+02	5.1E+03	0.0E+00	4.1E+04
174	3.2E+01	0.0E+00	2.8E+00	9.4E+01	1.3E+02	0.0E+00	3.9E+00	5.5E-01	0.0E+00	5.5E+00
175	1.3E+02	5.8E+00	2.3E+02	5.0E+00	1.0E+02	1.8E+00	1.7E+02	7.5E+01	1.9E+00	2.1E+01
176	6.4E+01	0.0E+00	1.1E+02	0.0E+00	1.5E+02	3.4E+00	7.4E+01	6.0E+02	5.9E-02	1.5E+01
177	1.9E+03	4.0E+01	5.8E+02	3.5E+02	1.4E+03	4.9E+01	3.3E+02	3.7E+03	0.0E+00	6.0E+02
178	1.9E+01	3.4E+00	1.1E+02	4.6E+00	3.9E+02	6.0E-01	2.7E+01	1.4E+02	0.0E+00	2.4E+00
179	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
180	0.0E+00	0.0E+00	0.0E+00	4.6E+00	1.9E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
181	3.6E+01	4.6E+00	3.2E+01	3.1E+00	1.5E+01	1.6E+00	1.2E+01	5.4E+00	3.9E-01	8.9E+00
182	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
183	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
184	7.6E+00	9.8E-01	6.8E+00	6.6E-01	3.2E+00	3.3E-01	2.5E+00	1.2E+00	8.2E-02	1.9E+00
185	4.9E+00	0.0E+00	3.8E+00	8.2E-01	6.0E+01	0.0E+00	0.0E+00	5.8E+00	0.0E+00	0.0E+00
186	4.1E+01	0.0E+00	1.3E+01	1.9E+01	2.2E+03	3.2E+00	0.0E+00	4.0E+01	0.0E+00	0.0E+00
187	2.5E+00	4.9E-02	9.3E+00	2.0E-01	1.7E-01	4.9E-02	4.6E+00	2.6E+00	7.4E-02	1.1E+00
188	2.9E+01	0.0E+00	7.7E+01	4.1E+00	6.5E+01	4.9E-01	5.2E+00	3.1E+01	3.9E-01	9.7E-02
189	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
190	9.1E+00	1.0E+00	2.7E+02	0.0E+00	5.0E+01	5.6E+00	2.1E+01	6.5E+01	1.1E+01	4.6E-01
191	1.8E+01	1.1E+00	2.5E+01	5.1E+00	1.7E+01	3.3E-01	1.9E+01	4.7E+01	0.0E+00	7.7E+00
192	6.3E+02	0.0E+00	0.0E+00	7.3E+01	9.4E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
193	3.7E+02	6.3E+00	1.2E+03	3.9E+01	3.9E+02	2.2E+00	2.7E+02	1.1E+03	1.4E+01	3.9E+01
194	1.3E+03	2.2E+01	4.3E+03	1.4E+02	1.4E+03	7.9E+00	9.7E+02	3.9E+03	5.0E+01	1.4E+02
195	1.1E+03	9.0E+02	3.1E+04	3.3E+01	2.8E+03	1.0E+02	3.6E+03	4.7E+03	1.2E+02	0.0E+00
196	6.2E+01	1.0E+01	1.4E+03	0.0E+00	9.4E+01	5.6E+00	8.3E+01	4.4E+02	3.1E+00	4.4E-01
197	2.3E+02	3.7E+01	5.2E+03	0.0E+00	3.4E+02	2.0E+01	3.0E+02	1.6E+03	1.1E+01	1.6E+00
198	4.8E+01	8.0E+00	1.1E+03	0.0E+00	7.2E+01	4.3E+00	6.4E+01	3.4E+02	2.4E+00	3.4E-01
199	8.8E+01	0.0E+00	3.6E+02	9.7E+01	1.0E+01	0.0E+00	4.3E+01	1.5E+02	0.0E+00	1.2E+02
200	2.2E+01	7.5E-02	9.9E+00	1.0E+00	2.6E+00	2.3E-01	1.5E+01	8.7E+00	5.6E-02	5.1E-01
201	1.4E-01	0.0E+00	0.0E+00	4.4E+00	2.7E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
202	1.0E+02	0.0E+00	0.0E+00	1.2E+01	1.5E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
203	3.1E+02	0.0E+00	2.4E+02	5.3E+01	3.9E+03	0.0E+00	0.0E+00	3.7E+02	0.0E+00	0.0E+00
204	8.8E+02	3.1E+00	4.1E+02	4.2E+01	1.0E+02	9.2E+00	6.3E+02	3.5E+02	2.3E+00	2.1E+01
205	4.6E+01	8.3E+00	1.8E+02	2.4E+01	2.2E+01	0.0E+00	7.2E+00	2.1E+02	8.7E+00	0.0E+00
206	4.4E-01	0.0E+00	0.0E+00	1.4E+01	8.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
207	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
208	0.0E+00	0.0E+00	0.0E+00	2.0E+00	8.1E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
209	8.6E+00	0.0E+00	1.8E+02	0.0E+00	1.5E+02	1.7E+00	8.7E+00	9.8E+01	2.1E-01	2.6E-01
210	7.5E+03	1.8E+02	1.6E+04	0.0E+00	1.8E+04	9.7E+01	2.0E+02	4.2E+03	1.6E+01	4.7E+00
211	1.8E-01	0.0E+00	0.0E+00	5.5E+00	3.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
212	1.6E+00	0.0E+00	0.0E+00	2.6E+01	3.8E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
213	0.0E+00	0.0E+00	0.0E+00	1.7E+01	7.1E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
214	1.9E+01	6.7E-02	8.9E+00	9.2E-01	2.3E+00	2.0E-01	1.4E+01	7.7E+00	5.0E-02	4.5E-01
215	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
216	3.0E+02	6.4E+01	7.2E+02	8.6E+01	2.8E+02	2.6E-01	1.9E+02	2.9E+02	1.4E+01	4.1E+01
217	6.2E+01	2.8E+00	1.1E+02	2.4E+00	5.0E+01	8.6E-01	8.5E+01	3.7E+01	9.1E-01	1.0E+01
218	2.9E+01	6.2E+00	7.0E+01	8.3E+00	2.7E+01	2.5E-02	1.8E+01	2.7E+01	1.4E+00	3.9E+00
219	1.3E+02	1.1E+02	3.7E+03	3.9E+00	3.2E+02	1.2E+01	4.2E+02	5.5E+02	1.5E+01	0.0E+00
220	8.6E+00	7.1E+00	2.5E+02	2.7E-01	2.2E+01	8.0E-01	2.9E+01	3.7E+01	9.8E-01	0.0E+00
221	2.8E+00	0.0E+00	1.1E+01	3.1E+00	3.2E-01	0.0E+00	1.4E+00	4.7E+00	0.0E+00	3.8E+00
222	5.8E+01	0.0E+00	1.8E+01	2.7E+01	3.1E+03	4.5E+00	0.0E+00	5.6E+01	0.0E+00	0.0E+00
223	5.0E+02	7.1E+01	1.2E+03	2.6E+02	1.4E+03	1.1E+00	5.9E+01	1.3E+03	3.6E-01	1.6E+00
224	3.0E+03	0.0E+00	4.3E+03	7.5E+02	5.5E+03	8.4E+01	1.0E+02	1.7E+03	1.6E+01	5.1E+02
225	2.0E+01	2.9E+00	4.8E+01	1.1E+01	5.6E+01	4.4E-02	2.4E+00	5.3E+01	1.5E-02	6.6E-02
226	1.5E+01	9.4E-01	5.3E+01	3.0E+00	4.2E+00	1.8E-01	5.4E+01	2.5E+01	0.0E+00	5.6E-01
227	2.6E+01	1.7E+00	9.4E+01	5.3E+00	7.4E+00	3.1E-01	9.7E+01	4.5E+01	0.0E+00	9.9E-01
228	1.3E+01	1.6E+00	5.2E-01	2.5E+01	7.3E+01	0.0E+00	5.2E-01	5.2E+00	0.0E+00	1.3E+01
229	3.2E+01	0.0E+00	2.5E+01	5.3E+00	3.9E+02	0.0E+00	0.0E+00	3.8E+01	0.0E+00	0.0E+00
230	6.4E-01	0.0E+00	0.0E+00	2.0E+01	1.2E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
231	2.9E-01	0.0E+00	0.0E+00	9.2E+00	5.7E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
232	1.9E+01	0.0E+00	7.7E+01	2.1E+01	2.2E+00	0.0E+00	9.2E+00	3.1E+01	0.0E+00	2.6E+01
233	3.3E+00	0.0E+00	0.0E+00	1.5E+00	8.5E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
234	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
235	9.9E+00	1.3E+00	8.9E+00	8.5E-01	4.2E+00	4.3E-01	3.3E+00	1.5E+00	1.1E-01	2.5E+00
236	1.4E+02	0.0E+00	2.0E+02	3.4E+01	2.5E+02	3.8E+00	4.7E+00	7.6E+01	7.1E-01	2.3E+01
237	1.0E+02	1.9E+01	4.0E+02	5.4E+01	4.9E+01	0.0E+00	1.6E+01	4.6E+02	1.9E+01	0.0E+00
238	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
239	9.7E+00	8.0E+00	2.8E+02	3.0E-01	2.5E+01	9.0E-01	3.3E+01	4.2E+01	1.1E+00	0.0E+00
240	7.4E+01	0.0E+00	1.3E+02	0.0E+00	1.8E+02	4.0E+00	8.6E+01	6.9E+02	6.9E-02	1.7E+01
241	7.5E+00	0.0E+00	3.0E+01	8.2E+00	8.6E-01	0.0E+00	3.6E+00	1.2E+01	0.0E+00	1.0E+01
242	6.3E+00	0.0E+00	1.1E+01	0.0E+00	1.5E+01	3.4E-01	7.3E+00	5.9E+01	5.8E-03	1.5E+00
243	3.6E+00	4.7E-01	3.2E+00	3.1E-01	1.5E+00	1.6E-01	1.2E+00	5.4E-01	3.9E-02	8.9E-01
244	2.3E+02	4.1E+01	1.3E+03	5.5E+01	4.7E+03	7.1E+00	3.3E+02	1.6E+03	0.0E+00	2.8E+01
245	2.3E-01	1.5E-01	5.5E+00	0.0E+00	1.8E-01	5.6E-02	1.1E-01	5.2E+00	3.1E-01	0.0E+00
246	4.6E-01	0.0E+00	0.0E+00	1.4E+01	8.8E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
247	4.1E+01	5.9E+00	9.8E+01	2.2E+01	1.1E+02	8.9E-02	4.8E+00	1.1E+02	3.0E-02	1.3E-01
248	2.1E+02	3.8E+01	8.3E+02	1.1E+02	1.0E+02	0.0E+00	3.3E+01	9.5E+02	4.0E+01	0.0E+00
249	7.3E+01	0.0E+00	2.3E+01	3.4E+01	3.9E+03	5.8E+00	0.0E+00	7.1E+01	0.0E+00	0.0E+00
250	2.6E-01	0.0E+00	0.0E+00	8.0E+00	5.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
251	2.8E-01	0.0E+00	2.6E+00	3.0E-02	4.2E-01	2.7E-01	5.0E-01	5.6E-01	0.0E+00	8.3E-01
252	1.1E+02	0.0E+00	8.7E+01	1.9E+01	1.4E+03	0.0E+00	0.0E+00	1.3E+02	0.0E+00	0.0E+00
253	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
254	1.7E+02	7.0E+00	6.6E+02	1.0E+02	1.5E+02	0.0E+00	1.3E+02	1.5E+02	0.0E+00	0.0E+00
255	1.2E+02	2.8E+00	2.5E+02	0.0E+00	2.9E+02	1.5E+00	3.1E+00	6.6E+01	2.5E-01	7.4E-02
256	2.2E+03	3.2E+02	5.3E+03	1.2E+03	6.1E+03	4.8E+00	2.6E+02	5.7E+03	1.6E+00	7.2E+00
257	2.5E+03	3.6E+02	6.0E+03	1.3E+03	6.9E+03	5.4E+00	3.0E+02	6.5E+03	1.8E+00	8.2E+00
258	1.9E+00	0.0E+00	1.7E+01	2.0E-01	2.8E+00	1.8E+00	3.3E+00	3.7E+00	0.0E+00	5.5E+00
259	8.2E+01	3.3E+00	3.1E+02	4.8E+01	7.3E+01	0.0E+00	6.4E+01	7.2E+01	0.0E+00	0.0E+00
260	9.6E-01	3.9E-02	3.7E+00	5.7E-01	8.5E-01	0.0E+00	7.5E-01	8.4E-01	0.0E+00	0.0E+00
261	0.0E+00	0.0E+00	2.8E+00	0.0E+00	5.3E-02	1.5E-02	1.4E+00	8.0E-01	2.3E-02	0.0E+00
262	4.0E+01	2.6E+00	1.5E+02	8.2E+00	1.2E+01	4.8E-01	1.5E+02	7.0E+01	0.0E+00	1.5E+00
263	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
264	4.2E+02	3.2E+01	2.2E+03	5.1E+01	2.3E+02	0.0E+00	7.5E+01	4.6E+03	5.4E+00	2.3E+01
265	2.1E+02	1.6E+01	1.1E+03	2.6E+01	1.2E+02	0.0E+00	3.8E+01	2.3E+03	2.7E+00	1.2E+01
266	1.3E+02	1.0E+01	7.1E+02	1.6E+01	7.4E+01	0.0E+00	2.4E+01	1.5E+03	1.7E+00	7.3E+00
267	2.4E+00	2.8E-02	3.5E+00	2.4E+00	3.9E+00	2.1E-01	1.8E-01	2.5E+00	1.6E-01	1.5E+00
268	1.4E+03	3.0E+02	3.3E+03	4.0E+02	1.3E+03	1.2E+00	8.6E+02	1.3E+03	6.4E+01	1.9E+02
269	3.2E+00	1.3E-01	1.2E+01	1.9E+00	2.9E+00	0.0E+00	2.5E+00	2.8E+00	0.0E+00	0.0E+00
270	5.1E+02	1.9E+02	3.9E+02	2.1E+02	5.1E+03	7.3E-01	1.8E+02	1.6E+03	9.0E+01	9.8E+00
271	4.2E+02	7.5E+01	2.4E+03	1.0E+02	8.7E+03	1.3E+01	6.0E+02	3.0E+03	0.0E+00	5.2E+01
272	1.4E+03	1.8E+02	1.7E+03	3.7E+02	4.2E+02	5.0E-01	1.8E+02	2.5E+03	1.0E+02	6.9E+01
273	1.6E+00	2.2E-01	3.3E+00	4.2E-01	4.5E+00	0.0E+00	5.2E-01	2.6E+00	1.4E-01	0.0E+00
274	3.0E-01	0.0E+00	0.0E+00	9.5E+00	5.9E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
275	4.8E+01	6.6E+00	9.7E+01	1.2E+01	1.4E+02	0.0E+00	1.6E+01	7.7E+01	4.2E+00	0.0E+00
276	3.1E+02	0.0E+00	4.5E+02	7.8E+01	5.8E+02	8.8E+00	1.1E+01	1.7E+02	1.6E+00	5.3E+01
277	8.2E-02	0.0E+00	7.6E-01	8.8E-03	1.2E-01	7.9E-02	1.5E-01	1.6E-01	0.0E+00	2.4E-01
278	7.6E+00	1.1E+00	7.4E+01	6.5E+00	1.1E+00	9.4E-01	1.7E+00	5.7E+01	5.0E+00	6.3E+00
279	5.9E+03	0.0E+00	8.4E+03	1.5E+03	1.1E+04	1.6E+02	2.0E+02	3.2E+03	3.0E+01	9.9E+02
280	6.9E+01	9.7E+00	6.6E+02	5.8E+01	9.5E+00	8.4E+00	1.6E+01	5.1E+02	4.5E+01	5.6E+01
281	1.5E+00	2.5E-01	3.4E+01	0.0E+00	2.2E+00	1.3E-01	2.0E+00	1.0E+01	7.4E-02	1.1E-02
282	2.0E+01	3.4E+00	4.6E+02	0.0E+00	3.0E+01	1.8E+00	2.7E+01	1.4E+02	1.0E+00	1.4E-01

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
283	4.1E+00	4.6E-01	1.2E+02	0.0E+00	2.3E+01	2.5E+00	9.3E+00	2.9E+01	4.9E+00	2.1E-01
284	2.0E+01	2.2E+00	5.8E+02	0.0E+00	1.1E+02	1.2E+01	4.6E+01	1.4E+02	2.4E+01	1.0E+00
285	8.6E+00	5.6E+00	4.2E+01	0.0E+00	5.7E+00	8.8E-02	2.9E+01	6.1E+01	0.0E+00	3.7E+00
286	2.3E+01	3.8E+00	5.3E+02	0.0E+00	3.4E+01	2.1E+00	3.1E+01	1.6E+02	1.1E+00	1.6E-01
287	1.6E+01	0.0E+00	3.4E+02	0.0E+00	2.7E+02	3.1E+00	1.6E+01	1.8E+02	3.9E-01	4.9E-01
288	2.7E+00	3.2E+00	9.2E+00	4.1E+00	1.0E+01	0.0E+00	1.1E+01	5.3E+01	0.0E+00	8.1E+00
289	2.7E+02	4.5E+00	8.5E+02	2.8E+01	2.8E+02	1.6E+00	1.9E+02	7.7E+02	1.0E+01	2.8E+01
290	2.3E+01	0.0E+00	1.2E+01	4.0E+00	3.1E+01	1.6E+01	1.1E+01	7.6E+01	0.0E+00	9.1E+00
291	4.4E+01	2.5E+00	6.0E+01	1.2E+01	4.1E+01	7.9E-01	4.5E+01	1.1E+02	0.0E+00	1.8E+01
292	2.1E+01	1.2E+00	2.8E+01	5.7E+00	1.9E+01	3.7E-01	2.1E+01	5.3E+01	0.0E+00	8.6E+00
293	1.6E+02	9.0E+00	2.2E+02	4.3E+01	1.5E+02	2.8E+00	1.6E+02	4.1E+02	0.0E+00	6.6E+01
294	3.5E+00	2.7E-01	1.9E+01	4.3E-01	2.0E+00	0.0E+00	6.3E-01	3.9E+01	4.6E-02	1.9E-01
295	2.3E+00	1.8E-01	1.3E+01	2.8E-01	1.3E+00	0.0E+00	4.2E-01	2.6E+01	3.1E-02	1.3E-01
296	1.4E+00	1.1E-01	7.5E+00	1.7E-01	7.8E-01	0.0E+00	2.5E-01	1.5E+01	1.8E-02	7.7E-02
297	6.9E+01	1.2E+00	2.2E+02	7.2E+00	7.2E+01	4.1E-01	5.0E+01	2.0E+02	2.6E+00	7.2E+00
298	1.7E+01	9.5E-01	2.3E+01	4.6E+00	1.6E+01	3.0E-01	1.7E+01	4.3E+01	0.0E+00	7.0E+00
299	1.8E-01	0.0E+00	0.0E+00	5.8E+00	3.6E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
300	9.0E+01	2.1E+00	1.9E+02	0.0E+00	2.2E+02	1.2E+00	2.4E+00	5.0E+01	1.9E-01	5.6E-02
301	1.1E+02	0.0E+00	1.5E+02	2.7E+01	2.0E+02	3.0E+00	3.7E+00	6.0E+01	5.6E-01	1.8E+01
302	1.9E+03	4.5E+01	3.9E+03	0.0E+00	4.6E+03	2.5E+01	5.0E+01	1.1E+03	3.9E+00	1.2E+00
303	1.1E-01	0.0E+00	0.0E+00	3.5E+00	2.2E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
304	2.0E+01	1.4E+01	4.9E+02	0.0E+00	1.6E+01	5.0E+00	9.7E+00	4.6E+02	2.8E+01	0.0E+00
305	3.1E+00	0.0E+00	0.0E+00	5.1E+01	7.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
306	2.6E+03	0.0E+00	1.2E+04	2.4E+02	2.4E+03	0.0E+00	0.0E+00	7.2E+03	0.0E+00	0.0E+00
307	6.5E+00	8.1E-01	2.7E-01	1.3E+01	3.8E+01	0.0E+00	2.7E-01	2.7E+00	0.0E+00	6.5E+00
308	1.5E+02	0.0E+00	3.9E+02	2.1E+01	3.3E+02	2.5E+00	2.6E+01	1.6E+02	2.0E+00	5.0E-01
309	1.1E+03	0.0E+00	5.0E+03	9.7E+01	9.7E+02	0.0E+00	0.0E+00	2.9E+03	0.0E+00	0.0E+00
310	2.0E+02	1.3E+01	7.2E+02	4.1E+01	5.7E+01	2.4E+00	7.4E+02	3.5E+02	0.0E+00	7.7E+00
311	1.9E+03	4.2E+02	4.7E+03	5.6E+02	1.8E+03	1.7E+00	1.2E+03	1.8E+03	9.0E+01	2.6E+02
312	4.7E-01	0.0E+00	4.4E+00	5.0E-02	7.0E-01	4.5E-01	8.4E-01	9.4E-01	0.0E+00	1.4E+00
313	4.8E+00	0.0E+00	0.0E+00	8.0E+01	1.2E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
314	6.0E+02	0.0E+00	2.8E+03	5.5E+01	5.5E+02	0.0E+00	0.0E+00	1.7E+03	0.0E+00	0.0E+00
315	2.2E+02	3.2E+01	5.3E+02	1.2E+02	6.2E+02	4.9E-01	2.6E+01	5.8E+02	1.6E-01	7.3E-01
316	3.1E-01	2.1E-01	7.6E+00	0.0E+00	2.4E-01	7.8E-02	1.5E-01	7.2E+00	4.4E-01	0.0E+00
317	4.7E+02	1.7E+02	3.7E+02	2.0E+02	4.7E+03	6.8E-01	1.6E+02	1.5E+03	8.4E+01	9.1E+00
318	1.1E-01	0.0E+00	0.0E+00	3.4E+00	2.1E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
319	5.1E-01	0.0E+00	0.0E+00	1.6E+01	9.8E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
320	9.4E+02	2.0E+02	2.3E+03	2.7E+02	8.7E+02	8.0E-01	5.8E+02	8.9E+02	4.4E+01	1.3E+02
321	4.0E-01	0.0E+00	0.0E+00	1.3E+01	7.7E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
322	4.1E-01	0.0E+00	0.0E+00	1.3E+01	8.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
323	3.4E+01	0.0E+00	1.0E+01	1.6E+01	1.8E+03	2.6E+00	0.0E+00	3.3E+01	0.0E+00	0.0E+00
324	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
325	7.6E+03	0.0E+00	1.1E+04	1.9E+03	1.4E+04	2.1E+02	2.6E+02	4.2E+03	3.9E+01	1.3E+03
326	2.3E-01	0.0E+00	0.0E+00	7.2E+00	4.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
327	5.3E-01	0.0E+00	1.6E-01	2.4E-01	2.8E+01	4.1E-02	0.0E+00	5.1E-01	0.0E+00	0.0E+00
328	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
329	1.7E+02	7.0E+00	6.6E+02	1.0E+02	1.5E+02	0.0E+00	1.3E+02	1.5E+02	0.0E+00	0.0E+00
330	2.6E+01	1.2E+00	4.6E+01	1.0E+00	2.1E+01	3.6E-01	3.5E+01	1.5E+01	3.8E-01	4.3E+00
331	3.7E+00	1.0E+00	1.9E+01	2.0E+00	1.8E+00	0.0E+00	2.2E-01	1.2E+01	0.0E+00	8.2E-01
332	7.5E+01	2.1E+01	3.8E+02	4.1E+01	3.6E+01	0.0E+00	4.4E+00	2.4E+02	0.0E+00	1.7E+01
333	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

Table D.11: .-Available irrigated area (ha/year) (Gónzalez, 2013; Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Alfalfa	Vetch	Barley	Corn Forage	Corn	Sorgo	Oat	Wheat	Rye	Barley Forage
334	6.2E+00	2.5E-01	2.4E+01	3.7E+00	5.5E+00	0.0E+00	4.8E+00	5.4E+00	0.0E+00	0.0E+00
335	2.0E+01	0.0E+00	8.2E+01	2.2E+01	2.3E+00	0.0E+00	9.8E+00	3.4E+01	0.0E+00	2.8E+01
336	8.6E+01	0.0E+00	3.5E+02	9.5E+01	9.9E+00	0.0E+00	4.2E+01	1.4E+02	0.0E+00	1.2E+02
337	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
338	1.5E+03	0.0E+00	4.1E+03	2.2E+02	3.5E+03	2.6E+01	2.8E+02	1.6E+03	2.1E+01	5.2E+00
339	8.1E+01	5.3E+01	3.9E+02	0.0E+00	5.4E+01	8.4E-01	2.8E+02	5.8E+02	0.0E+00	3.5E+01
340	1.0E+01	0.0E+00	0.0E+00	4.8E+00	2.7E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
341	1.1E-01	0.0E+00	0.0E+00	3.4E+00	2.1E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
342	1.9E+02	6.6E-01	8.7E+01	9.1E+00	2.2E+01	2.0E+00	1.4E+02	7.6E+01	4.9E-01	4.5E+00
343	1.6E+00	2.8E-01	8.7E+00	3.7E-01	3.2E+01	4.9E-02	2.2E+00	1.1E+01	0.0E+00	1.9E-01
344	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
345	1.3E+04	4.1E+01	1.3E+04	0.0E+00	5.5E+03	1.0E+02	1.7E+02	1.1E+04	3.5E+01	1.1E+00

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
1	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
2	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
3	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
4	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
5	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
6	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
7	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
8	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
9	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
10	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
11	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
12	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
13	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
14	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
15	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
16	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
17	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
18	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
19	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
20	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
21	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
22	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
23	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
24	1.7E+03	1.2E+03	1.3E+03	8.4E+02	6.0E+03	2.0E+03	2.9E+03	0.0E+00	3.0E+04	1.7E+04	9.1E+03	2.1E
25	1.6E+03	1.0E+03	1.4E+03	9.4E+02	6.0E+03	2.1E+03	1.6E+03	0.0E+00	2.9E+04	1.6E+04	8.9E+03	0.0E
26	1.6E+03	1.0E+03	1.4E+03	9.4E+02	6.0E+03	2.1E+03	1.6E+03	0.0E+00	2.9E+04	1.6E+04	8.9E+03	0.0E
27	1.6E+03	1.0E+03	1.4E+03	9.4E+02	6.0E+03	2.1E+03	1.6E+03	0.0E+00	2.9E+04	1.6E+04	8.9E+03	0.0E
28	1.6E+03	1.0E+03	1.4E+03	9.4E+02	6.0E+03	2.1E+03	1.6E+03	0.0E+00	2.9E+04	1.6E+04	8.9E+03	0.0E
29	1.6E+03	1.0E+03	1.4E+03	9.4E+02	6.0E+03	2.1E+03	1.6E+03	0.0E+00	2.9E+04	1.6E+04	8.9E+03	0.0E
30	1.7E+03	1.1E+03	1.4E+03	9.0E+02	6.5E+03	3.1E+03	4.0E+03	0.0E+00	2.9E+04	1.7E+04	8.9E+03	2.5E
31	1.7E+03	1.1E+03	1.4E+03	9.0E+02	6.5E+03	3.1E+03	4.0E+03	0.0E+00	2.9E+04	1.7E+04	8.9E+03	2.5E
32	1.7E+03	1.1E+03	1.4E+03	9.0E+02	6.5E+03	3.1E+03	4.0E+03	0.0E+00	2.9E+04	1.7E+04	8.9E+03	2.5E
33	1.3E+03	8.8E+02	1.2E+03	7.8E+02	4.9E+03	2.2E+03	2.1E+03	0.0E+00	3.2E+04	1.9E+04	0.0E+00	2.5E

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
34	1.3E+03	8.8E+02	1.2E+03	7.8E+02	4.9E+03	2.2E+03	2.1E+03	0.0E+00	3.2E+04	1.9E+04	0.0E+00	2.5E+04
35	1.3E+03	8.8E+02	1.2E+03	7.8E+02	4.9E+03	2.2E+03	2.1E+03	0.0E+00	3.2E+04	1.9E+04	0.0E+00	2.5E+04
36	1.3E+03	8.8E+02	1.2E+03	7.8E+02	4.9E+03	2.2E+03	2.1E+03	0.0E+00	3.2E+04	1.9E+04	0.0E+00	2.5E+04
37	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
38	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
39	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
40	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
41	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
42	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
43	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
44	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
45	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
46	1.2E+03	8.0E+02	0.0E+00	0.0E+00	2.6E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	0.0E+00	3.2E+04	0.0E+00
47	1.3E+03	8.5E+02	1.0E+03	6.8E+02	1.5E+03	1.4E+03	1.3E+03	0.0E+00	5.5E+04	1.5E+04	1.3E+04	1.2E+04
48	1.3E+03	8.5E+02	1.0E+03	6.8E+02	1.5E+03	1.4E+03	1.3E+03	0.0E+00	5.5E+04	1.5E+04	1.3E+04	1.2E+04
49	1.3E+03	8.5E+02	1.0E+03	6.8E+02	1.5E+03	1.4E+03	1.3E+03	0.0E+00	5.5E+04	1.5E+04	1.3E+04	1.2E+04
50	1.3E+03	8.5E+02	1.0E+03	6.8E+02	1.5E+03	1.4E+03	1.3E+03	0.0E+00	5.5E+04	1.5E+04	1.3E+04	1.2E+04
51	1.3E+03	8.5E+02	1.0E+03	6.8E+02	1.5E+03	1.4E+03	1.3E+03	0.0E+00	5.5E+04	1.5E+04	1.3E+04	1.2E+04
52	1.3E+03	8.5E+02	1.0E+03	6.8E+02	1.5E+03	1.4E+03	1.3E+03	0.0E+00	5.5E+04	1.5E+04	1.3E+04	1.2E+04
53	4.1E+03	2.7E+03	4.2E+03	2.8E+03	4.7E+03	5.5E+03	5.5E+03	0.0E+00	3.5E+04	2.6E+04	4.3E+04	2.2E+04
54	4.1E+03	2.7E+03	4.2E+03	2.8E+03	4.7E+03	5.5E+03	5.5E+03	0.0E+00	3.5E+04	2.6E+04	4.3E+04	2.2E+04
55	4.1E+03	2.7E+03	4.2E+03	2.8E+03	4.7E+03	5.5E+03	5.5E+03	0.0E+00	3.5E+04	2.6E+04	4.3E+04	2.2E+04
56	4.1E+03	2.7E+03	4.2E+03	2.8E+03	4.7E+03	5.5E+03	5.5E+03	0.0E+00	3.5E+04	2.6E+04	4.3E+04	2.2E+04
57	4.1E+03	2.7E+03	4.2E+03	2.8E+03	4.7E+03	5.5E+03	5.5E+03	0.0E+00	3.5E+04	2.6E+04	4.3E+04	2.2E+04
58	4.1E+03	2.7E+03	4.2E+03	2.8E+03	4.7E+03	5.5E+03	5.5E+03	0.0E+00	3.5E+04	2.6E+04	4.3E+04	2.2E+04
59	3.3E+03	2.2E+03	0.0E+00	0.0E+00	3.2E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	2.0E+04	4.1E+04	2.6E+04
60	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.4E+03	0.0E+00	0.0E+00	0.0E+00	4.2E+04	2.4E+04	4.1E+04	2.6E+04
61	3.1E+03	2.1E+03	2.3E+03	1.6E+03	5.9E+03	4.8E+03	2.8E+03	0.0E+00	3.3E+04	1.6E+04	1.4E+04	1.6E+04
62	3.1E+03	2.1E+03	2.3E+03	1.6E+03	5.9E+03	4.8E+03	2.8E+03	0.0E+00	3.3E+04	1.6E+04	1.4E+04	1.6E+04
63	3.1E+03	2.1E+03	2.3E+03	1.6E+03	5.9E+03	4.8E+03	2.8E+03	0.0E+00	3.3E+04	1.6E+04	1.4E+04	1.6E+04
64	3.1E+03	2.1E+03	2.3E+03	1.6E+03	5.9E+03	4.8E+03	2.8E+03	0.0E+00	3.3E+04	1.6E+04	1.4E+04	1.6E+04
65	3.1E+03	2.1E+03	2.3E+03	1.6E+03	5.9E+03	4.8E+03	2.8E+03	0.0E+00	3.3E+04	1.6E+04	1.4E+04	1.6E+04
66	3.1E+03	2.1E+03	2.3E+03	1.6E+03	5.9E+03	4.8E+03	2.8E+03	0.0E+00	3.3E+04	1.6E+04	1.4E+04	1.6E+04
67	3.1E+03	2.1E+03	2.3E+03	1.6E+03	5.9E+03	4.8E+03	2.8E+03	0.0E+00	3.3E+04	1.6E+04	1.4E+04	1.6E+04
68	2.9E+03	1.9E+03	2.8E+03	1.8E+03	0.0E+00	4.1E+03	3.6E+03	0.0E+00	0.0E+00	1.5E+04	2.0E+04	1.6E+04
69	2.9E+03	1.9E+03	2.8E+03	1.8E+03	0.0E+00	4.1E+03	3.6E+03	0.0E+00	0.0E+00	1.5E+04	2.0E+04	1.6E+04
70	2.9E+03	1.9E+03	2.8E+03	1.8E+03	0.0E+00	4.1E+03	3.6E+03	0.0E+00	0.0E+00	1.5E+04	2.0E+04	1.6E+04
71	2.9E+03	1.9E+03	2.8E+03	1.8E+03	0.0E+00	4.1E+03	3.6E+03	0.0E+00	0.0E+00	1.5E+04	2.0E+04	1.6E+04
72	2.9E+03	1.9E+03	2.8E+03	1.8E+03	0.0E+00	4.1E+03	3.6E+03	0.0E+00	0.0E+00	1.5E+04	2.0E+04	1.6E+04
73	2.9E+03	1.9E+03	2.8E+03	1.8E+03	0.0E+00	4.1E+03	3.6E+03	0.0E+00	0.0E+00	1.5E+04	2.0E+04	1.6E+04
74	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
75	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
76	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
77	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
78	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
79	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
80	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
81	2.0E+03	1.3E+03	1.8E+03	1.2E+03	0.0E+00	2.7E+03	2.8E+03	9.0E+02	3.3E+04	1.1E+04	2.2E+04	1.8E+04
82	1.0E+03	6.7E+02	1.2E+03	8.1E+02	0.0E+00	1.5E+03	2.4E+03	0.0E+00	1.3E+04	7.1E+03	4.8E+03	7.5E+03
83	1.0E+03	6.7E+02	1.2E+03	8.1E+02	0.0E+00	1.5E+03	2.4E+03	0.0E+00	1.3E+04	7.1E+03	4.8E+03	7.5E+03
84	1.0E+03	6.7E+02	1.2E+03	8.1E+02	0.0E+00	1.5E+03	2.4E+03	0.0E+00	1.3E+04	7.1E+03	4.8E+03	7.5E+03

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
85	1.0E+03	6.7E+02	1.2E+03	8.1E+02	0.0E+00	1.5E+03	2.4E+03	0.0E+00	1.3E+04	7.1E+03	4.8E+03	7.5E
86	1.0E+03	6.7E+02	1.2E+03	8.1E+02	0.0E+00	1.5E+03	2.4E+03	0.0E+00	1.3E+04	7.1E+03	4.8E+03	7.5E
87	1.0E+03	6.7E+02	1.2E+03	8.1E+02	0.0E+00	1.5E+03	2.4E+03	0.0E+00	1.3E+04	7.1E+03	4.8E+03	7.5E
88	1.1E+03	7.1E+02	1.2E+03	8.2E+02	6.5E+03	1.5E+03	1.6E+03	3.1E+03	0.0E+00	8.0E+03	1.5E+04	1.0E
89	1.1E+03	7.1E+02	1.2E+03	8.2E+02	6.5E+03	1.5E+03	1.6E+03	3.1E+03	0.0E+00	8.0E+03	1.5E+04	1.0E
90	1.1E+03	7.1E+02	1.2E+03	8.2E+02	6.5E+03	1.5E+03	1.6E+03	3.1E+03	0.0E+00	8.0E+03	1.5E+04	1.0E
91	1.1E+03	7.1E+02	1.2E+03	8.2E+02	6.5E+03	1.5E+03	1.6E+03	3.1E+03	0.0E+00	8.0E+03	1.5E+04	1.0E
92	1.1E+03	7.1E+02	1.2E+03	8.2E+02	6.5E+03	1.5E+03	1.6E+03	3.1E+03	0.0E+00	8.0E+03	1.5E+04	1.0E
93	1.1E+03	7.1E+02	1.2E+03	8.2E+02	6.5E+03	1.5E+03	1.6E+03	3.1E+03	0.0E+00	8.0E+03	1.5E+04	1.0E
94	1.1E+03	7.1E+02	1.2E+03	8.2E+02	6.5E+03	1.5E+03	1.6E+03	3.1E+03	0.0E+00	8.0E+03	1.5E+04	1.0E
95	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
96	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
97	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
98	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
99	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
100	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
101	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
102	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
103	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
104	2.5E+03	1.6E+03	2.2E+03	1.5E+03	5.0E+03	2.6E+03	3.5E+03	0.0E+00	3.6E+04	1.4E+04	1.7E+04	0.0E
105	2.4E+03	1.6E+03	2.5E+03	1.6E+03	5.3E+03	2.1E+03	2.5E+03	3.6E+03	3.8E+04	1.6E+04	1.5E+04	1.5E
106	2.4E+03	1.6E+03	2.5E+03	1.6E+03	5.3E+03	2.1E+03	2.5E+03	3.6E+03	3.8E+04	1.6E+04	1.5E+04	1.5E
107	2.4E+03	1.6E+03	2.5E+03	1.6E+03	5.3E+03	2.1E+03	2.5E+03	3.6E+03	3.8E+04	1.6E+04	1.5E+04	1.5E
108	2.4E+03	1.6E+03	2.5E+03	1.6E+03	5.3E+03	2.1E+03	2.5E+03	3.6E+03	3.8E+04	1.6E+04	1.5E+04	1.5E
109	2.4E+03	1.6E+03	2.5E+03	1.6E+03	5.3E+03	2.1E+03	2.5E+03	3.6E+03	3.8E+04	1.6E+04	1.5E+04	1.5E
110	2.4E+03	1.6E+03	2.5E+03	1.6E+03	5.3E+03	2.1E+03	2.5E+03	3.6E+03	3.8E+04	1.6E+04	1.5E+04	1.5E
111	2.4E+03	1.6E+03	2.5E+03	1.6E+03	5.3E+03	2.1E+03	2.5E+03	3.6E+03	3.8E+04	1.6E+04	1.5E+04	1.5E
112	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
113	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
114	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
115	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
116	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
117	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
118	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
119	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
120	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
121	1.6E+03	1.1E+03	1.5E+03	9.7E+02	4.4E+03	2.3E+03	1.8E+03	2.9E+03	1.8E+04	1.2E+04	1.6E+04	1.5E
122	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
123	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
124	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
125	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
126	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
127	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
128	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
129	1.7E+03	1.1E+03	1.4E+03	9.0E+02	4.0E+03	5.6E+02	5.0E+02	1.5E+03	0.0E+00	8.0E+03	1.8E+04	0.0E
130	9.1E+02	6.0E+02	8.2E+02	5.5E+02	0.0E+00	5.5E+02	9.0E+02	0.0E+00	0.0E+00	1.1E+04	0.0E+00	9.5E
131	9.1E+02	6.0E+02	8.2E+02	5.5E+02	0.0E+00	5.5E+02	9.0E+02	0.0E+00	0.0E+00	1.1E+04	0.0E+00	9.5E
132	9.1E+02	6.0E+02	8.2E+02	5.5E+02	0.0E+00	5.5E+02	9.0E+02	0.0E+00	0.0E+00	1.1E+04	0.0E+00	9.5E
133	8.2E+02	5.4E+02	7.4E+02	5.0E+02	0.0E+00	7.6E+02	8.8E+02	0.0E+00	0.0E+00	9.4E+03	1.7E+04	1.1E
134	8.2E+02	5.4E+02	7.4E+02	5.0E+02	0.0E+00	7.6E+02	8.8E+02	0.0E+00	0.0E+00	9.4E+03	1.7E+04	1.1E
135	8.2E+02	5.4E+02	7.4E+02	5.0E+02	0.0E+00	7.6E+02	8.8E+02	0.0E+00	0.0E+00	9.4E+03	1.7E+04	1.1E

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
136	8.2E+02	5.4E+02	7.4E+02	5.0E+02	0.0E+00	7.6E+02	8.8E+02	0.0E+00	0.0E+00	9.4E+03	1.7E+04	1.1E+04
137	8.2E+02	5.4E+02	7.4E+02	5.0E+02	0.0E+00	7.6E+02	8.8E+02	0.0E+00	0.0E+00	9.4E+03	1.7E+04	1.1E+04
138	8.2E+02	5.4E+02	7.4E+02	5.0E+02	0.0E+00	7.6E+02	8.8E+02	0.0E+00	0.0E+00	9.4E+03	1.7E+04	1.1E+04
139	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
140	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
141	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
142	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
143	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
144	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
145	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
146	2.2E+03	1.5E+03	2.4E+03	1.6E+03	0.0E+00	3.2E+03	2.6E+03	0.0E+00	2.0E+04	1.5E+04	2.0E+04	1.7E+04
147	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
148	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
149	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
150	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
151	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
152	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
153	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
154	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
155	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
156	9.9E+02	6.6E+02	1.1E+03	7.2E+02	0.0E+00	9.5E+02	1.2E+03	0.0E+00	0.0E+00	1.0E+04	1.6E+04	8.0E+03
157	1.6E+03	1.1E+03	1.7E+03	1.1E+03	0.0E+00	2.6E+03	2.5E+03	0.0E+00	0.0E+00	8.8E+03	2.2E+04	1.8E+04
158	1.6E+03	1.1E+03	1.7E+03	1.1E+03	0.0E+00	2.6E+03	2.5E+03	0.0E+00	0.0E+00	8.8E+03	2.2E+04	1.8E+04
159	1.6E+03	1.1E+03	1.7E+03	1.1E+03	0.0E+00	2.6E+03	2.5E+03	0.0E+00	0.0E+00	8.8E+03	2.2E+04	1.8E+04
160	1.6E+03	1.1E+03	1.7E+03	1.1E+03	0.0E+00	2.6E+03	2.5E+03	0.0E+00	0.0E+00	8.8E+03	2.2E+04	1.8E+04
161	1.6E+03	1.1E+03	1.7E+03	1.1E+03	0.0E+00	2.6E+03	2.5E+03	0.0E+00	0.0E+00	8.8E+03	2.2E+04	1.8E+04
162	1.6E+03	1.1E+03	1.7E+03	1.1E+03	0.0E+00	2.6E+03	2.5E+03	0.0E+00	0.0E+00	8.8E+03	2.2E+04	1.8E+04
163	1.6E+03	1.1E+03	1.7E+03	1.1E+03	0.0E+00	2.6E+03	2.5E+03	0.0E+00	0.0E+00	8.8E+03	2.2E+04	1.8E+04
164	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
165	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
166	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
167	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
168	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
169	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
170	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
171	9.8E+02	6.6E+02	9.6E+02	6.4E+02	0.0E+00	1.1E+03	1.0E+03	3.0E+03	0.0E+00	1.0E+04	2.0E+04	9.0E+03
172	1.3E+03	8.4E+02	1.4E+03	9.2E+02	0.0E+00	1.5E+03	1.7E+03	0.0E+00	0.0E+00	1.5E+04	0.0E+00	1.4E+04
173	1.3E+03	8.4E+02	1.4E+03	9.2E+02	0.0E+00	1.5E+03	1.7E+03	0.0E+00	0.0E+00	1.5E+04	0.0E+00	1.4E+04
174	1.3E+03	8.4E+02	1.4E+03	9.2E+02	0.0E+00	1.5E+03	1.7E+03	0.0E+00	0.0E+00	1.5E+04	0.0E+00	1.4E+04
175	1.8E+03	1.2E+03	1.9E+03	1.3E+03	0.0E+00	1.6E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	1.5E+04	1.6E+04
176	1.8E+03	1.2E+03	1.9E+03	1.3E+03	0.0E+00	1.6E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	1.5E+04	1.6E+04
177	1.8E+03	1.2E+03	1.9E+03	1.3E+03	0.0E+00	1.6E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	1.5E+04	1.6E+04
178	1.8E+03	1.2E+03	1.9E+03	1.3E+03	0.0E+00	1.6E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	1.5E+04	1.6E+04
179	1.8E+03	1.2E+03	1.9E+03	1.3E+03	0.0E+00	1.6E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	1.5E+04	1.6E+04
180	1.8E+03	1.2E+03	1.9E+03	1.3E+03	0.0E+00	1.6E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	1.5E+04	1.6E+04
181	1.8E+03	1.2E+03	1.9E+03	1.3E+03	0.0E+00	1.6E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	1.5E+04	1.6E+04
182	1.1E+03	7.1E+02	1.4E+03	9.0E+02	0.0E+00	1.1E+03	1.1E+03	0.0E+00	0.0E+00	1.0E+04	1.5E+04	1.4E+04
183	1.1E+03	7.1E+02	1.4E+03	9.0E+02	0.0E+00	1.1E+03	1.1E+03	0.0E+00	0.0E+00	1.0E+04	1.5E+04	1.4E+04
184	1.1E+03	7.1E+02	1.4E+03	9.0E+02	0.0E+00	1.1E+03	1.1E+03	0.0E+00	0.0E+00	1.0E+04	1.5E+04	1.4E+04
185	1.1E+03	7.1E+02	1.4E+03	9.0E+02	0.0E+00	1.1E+03	1.1E+03	0.0E+00	0.0E+00	1.0E+04	1.5E+04	1.4E+04
186	1.3E+03	8.8E+02	1.4E+03	9.4E+02	0.0E+00	1.4E+03	1.7E+03	0.0E+00	0.0E+00	1.2E+04	1.5E+04	1.6E+04

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
187	1.3E+03	8.8E+02	1.4E+03	9.4E+02	0.0E+00	1.4E+03	1.7E+03	0.0E+00	0.0E+00	1.2E+04	1.5E+04	1.6E
188	1.3E+03	8.8E+02	1.4E+03	9.4E+02	0.0E+00	1.4E+03	1.7E+03	0.0E+00	0.0E+00	1.2E+04	1.5E+04	1.6E
189	1.3E+03	8.8E+02	1.4E+03	9.4E+02	0.0E+00	1.4E+03	1.7E+03	0.0E+00	0.0E+00	1.2E+04	1.5E+04	1.6E
190	1.3E+03	8.8E+02	1.4E+03	9.4E+02	0.0E+00	1.4E+03	1.7E+03	0.0E+00	0.0E+00	1.2E+04	1.5E+04	1.6E
191	1.3E+03	8.8E+02	1.4E+03	9.4E+02	0.0E+00	1.4E+03	1.7E+03	0.0E+00	0.0E+00	1.2E+04	1.5E+04	1.6E
192	1.0E+03	6.7E+02	1.1E+03	7.1E+02	1.2E+04	9.8E+02	1.2E+03	1.4E+03	0.0E+00	1.3E+04	2.3E+04	0.0E
193	1.0E+03	6.7E+02	1.1E+03	7.1E+02	1.2E+04	9.8E+02	1.2E+03	1.4E+03	0.0E+00	1.3E+04	2.3E+04	0.0E
194	1.0E+03	6.7E+02	1.1E+03	7.1E+02	1.2E+04	9.8E+02	1.2E+03	1.4E+03	0.0E+00	1.3E+04	2.3E+04	0.0E
195	1.0E+03	6.7E+02	1.1E+03	7.1E+02	1.2E+04	9.8E+02	1.2E+03	1.4E+03	0.0E+00	1.3E+04	2.3E+04	0.0E
196	1.0E+03	6.7E+02	1.1E+03	7.1E+02	1.2E+04	9.8E+02	1.2E+03	1.4E+03	0.0E+00	1.3E+04	2.3E+04	0.0E
197	1.0E+03	6.7E+02	1.1E+03	7.1E+02	1.2E+04	9.8E+02	1.2E+03	1.4E+03	0.0E+00	1.3E+04	2.3E+04	0.0E
198	1.3E+03	8.8E+02	1.4E+03	9.6E+02	0.0E+00	1.9E+03	1.3E+03	0.0E+00	0.0E+00	3.6E+03	0.0E+00	1.0E
199	1.3E+03	8.8E+02	1.4E+03	9.6E+02	0.0E+00	1.9E+03	1.3E+03	0.0E+00	0.0E+00	3.6E+03	0.0E+00	1.0E
200	1.3E+03	8.8E+02	1.4E+03	9.6E+02	0.0E+00	1.9E+03	1.3E+03	0.0E+00	0.0E+00	3.6E+03	0.0E+00	1.0E
201	1.3E+03	8.8E+02	1.4E+03	9.6E+02	0.0E+00	1.9E+03	1.3E+03	0.0E+00	0.0E+00	3.6E+03	0.0E+00	1.0E
202	1.3E+03	8.8E+02	1.4E+03	9.6E+02	0.0E+00	1.9E+03	1.3E+03	0.0E+00	0.0E+00	3.6E+03	0.0E+00	1.0E
203	1.3E+03	8.8E+02	1.4E+03	9.6E+02	0.0E+00	1.9E+03	1.3E+03	0.0E+00	0.0E+00	3.6E+03	0.0E+00	1.0E
204	1.3E+03	8.8E+02	1.4E+03	9.6E+02	0.0E+00	1.9E+03	1.3E+03	0.0E+00	0.0E+00	3.6E+03	0.0E+00	1.0E
205	9.7E+02	6.5E+02	1.1E+03	7.3E+02	9.0E+02	1.7E+03	1.0E+03	1.7E+03	0.0E+00	1.3E+04	0.0E+00	3.7E
206	9.7E+02	6.5E+02	1.1E+03	7.3E+02	9.0E+02	1.7E+03	1.0E+03	1.7E+03	0.0E+00	1.3E+04	0.0E+00	3.7E
207	9.7E+02	6.5E+02	1.1E+03	7.3E+02	9.0E+02	1.7E+03	1.0E+03	1.7E+03	0.0E+00	1.3E+04	0.0E+00	3.7E
208	9.7E+02	6.5E+02	1.1E+03	7.3E+02	9.0E+02	1.7E+03	1.0E+03	1.7E+03	0.0E+00	1.3E+04	0.0E+00	3.7E
209	9.7E+02	6.5E+02	1.1E+03	7.3E+02	9.0E+02	1.7E+03	1.0E+03	1.7E+03	0.0E+00	1.3E+04	0.0E+00	3.7E
210	9.7E+02	6.5E+02	1.1E+03	7.3E+02	9.0E+02	1.7E+03	1.0E+03	1.7E+03	0.0E+00	1.3E+04	0.0E+00	3.7E
211	1.3E+03	8.8E+02	1.4E+03	9.2E+02	3.8E+03	2.0E+03	1.8E+03	1.4E+03	0.0E+00	3.0E+03	1.3E+04	1.0E
212	1.3E+03	8.8E+02	1.4E+03	9.2E+02	3.8E+03	2.0E+03	1.8E+03	1.4E+03	0.0E+00	3.0E+03	1.3E+04	1.0E
213	1.3E+03	8.8E+02	1.4E+03	9.2E+02	3.8E+03	2.0E+03	1.8E+03	1.4E+03	0.0E+00	3.0E+03	1.3E+04	1.0E
214	1.3E+03	8.8E+02	1.4E+03	9.2E+02	3.8E+03	2.0E+03	1.8E+03	1.4E+03	0.0E+00	3.0E+03	1.3E+04	1.0E
215	1.3E+03	8.8E+02	1.4E+03	9.2E+02	3.8E+03	2.0E+03	1.8E+03	1.4E+03	0.0E+00	3.0E+03	1.3E+04	1.0E
216	1.3E+03	8.8E+02	1.4E+03	9.2E+02	3.8E+03	2.0E+03	1.8E+03	1.4E+03	0.0E+00	3.0E+03	1.3E+04	1.0E
217	1.3E+03	8.8E+02	1.4E+03	9.2E+02	3.8E+03	2.0E+03	1.8E+03	1.4E+03	0.0E+00	3.0E+03	1.3E+04	1.0E
218	1.7E+03	1.1E+03	1.7E+03	1.1E+03	7.0E+03	1.5E+03	1.0E+03	0.0E+00	0.0E+00	7.0E+03	3.0E+04	9.0E
219	1.7E+03	1.1E+03	1.7E+03	1.1E+03	7.0E+03	1.5E+03	1.0E+03	0.0E+00	0.0E+00	7.0E+03	3.0E+04	9.0E
220	1.7E+03	1.1E+03	1.7E+03	1.1E+03	7.0E+03	1.5E+03	1.0E+03	0.0E+00	0.0E+00	7.0E+03	3.0E+04	9.0E
221	1.7E+03	1.1E+03	1.7E+03	1.1E+03	7.0E+03	1.5E+03	1.0E+03	0.0E+00	0.0E+00	7.0E+03	3.0E+04	9.0E
222	1.7E+03	1.1E+03	1.7E+03	1.1E+03	7.0E+03	1.5E+03	1.0E+03	0.0E+00	0.0E+00	7.0E+03	3.0E+04	9.0E
223	7.4E+02	4.9E+02	7.6E+02	5.0E+02	0.0E+00	4.4E+02	7.0E+02	1.4E+03	0.0E+00	1.1E+04	2.3E+04	1.6E
224	7.4E+02	4.9E+02	7.6E+02	5.0E+02	0.0E+00	4.4E+02	7.0E+02	1.4E+03	0.0E+00	1.1E+04	2.3E+04	1.6E
225	7.4E+02	4.9E+02	7.6E+02	5.0E+02	0.0E+00	4.4E+02	7.0E+02	1.4E+03	0.0E+00	1.1E+04	2.3E+04	1.6E
226	7.4E+02	4.9E+02	7.6E+02	5.0E+02	0.0E+00	4.4E+02	7.0E+02	1.4E+03	0.0E+00	1.1E+04	2.3E+04	1.6E
227	7.4E+02	4.9E+02	7.6E+02	5.0E+02	0.0E+00	4.4E+02	7.0E+02	1.4E+03	0.0E+00	1.1E+04	2.3E+04	1.6E
228	7.4E+02	4.9E+02	7.6E+02	5.0E+02	0.0E+00	4.4E+02	7.0E+02	1.4E+03	0.0E+00	1.1E+04	2.3E+04	1.6E
229	7.4E+02	4.9E+02	7.6E+02	5.0E+02	0.0E+00	4.4E+02	7.0E+02	1.4E+03	0.0E+00	1.1E+04	2.3E+04	1.6E
230	6.6E+02	4.4E+02	5.7E+02	3.8E+02	0.0E+00	8.5E+02	4.5E+02	2.0E+03	0.0E+00	4.0E+03	6.0E+03	5.5E
231	6.6E+02	4.4E+02	5.7E+02	3.8E+02	0.0E+00	8.5E+02	4.5E+02	2.0E+03	0.0E+00	4.0E+03	6.0E+03	5.5E
232	6.6E+02	4.4E+02	5.7E+02	3.8E+02	0.0E+00	8.5E+02	4.5E+02	2.0E+03	0.0E+00	4.0E+03	6.0E+03	5.5E
233	6.6E+02	4.4E+02	5.7E+02	3.8E+02	0.0E+00	8.5E+02	4.5E+02	2.0E+03	0.0E+00	4.0E+03	6.0E+03	5.5E
234	6.6E+02	4.4E+02	5.7E+02	3.8E+02	0.0E+00	8.5E+02	4.5E+02	2.0E+03	0.0E+00	4.0E+03	6.0E+03	5.5E
235	9.6E+02	6.4E+02	8.3E+02	5.6E+02	2.1E+03	1.2E+03	9.4E+02	2.2E+03	3.8E+03	1.7E+03	8.0E+03	2.0E
236	9.6E+02	6.4E+02	8.3E+02	5.6E+02	2.1E+03	1.2E+03	9.4E+02	2.2E+03	3.8E+03	1.7E+03	8.0E+03	2.0E
237	9.6E+02	6.4E+02	8.3E+02	5.6E+02	2.1E+03	1.2E+03	9.4E+02	2.2E+03	3.8E+03	1.7E+03	8.0E+03	2.0E

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
238	9.6E+02	6.4E+02	8.3E+02	5.6E+02	2.1E+03	1.2E+03	9.4E+02	2.2E+03	3.8E+03	1.7E+03	8.0E+03	2.0E+03
239	9.6E+02	6.4E+02	8.3E+02	5.6E+02	2.1E+03	1.2E+03	9.4E+02	2.2E+03	3.8E+03	1.7E+03	8.0E+03	2.0E+03
240	9.6E+02	6.4E+02	8.3E+02	5.6E+02	2.1E+03	1.2E+03	9.4E+02	2.2E+03	3.8E+03	1.7E+03	8.0E+03	2.0E+03
241	9.6E+02	6.4E+02	8.3E+02	5.6E+02	2.1E+03	1.2E+03	9.4E+02	2.2E+03	3.8E+03	1.7E+03	8.0E+03	2.0E+03
242	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
243	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
244	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
245	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
246	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
247	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
248	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
249	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
250	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
251	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
252	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
253	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
254	8.1E+02	5.4E+02	8.7E+02	5.8E+02	0.0E+00	1.3E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	6.5E+02
255	6.9E+02	4.6E+02	7.8E+02	5.2E+02	2.0E+03	1.3E+03	5.3E+02	8.9E+02	3.8E+03	3.0E+03	0.0E+00	1.8E+03
256	6.9E+02	4.6E+02	7.8E+02	5.2E+02	2.0E+03	1.3E+03	5.3E+02	8.9E+02	3.8E+03	3.0E+03	0.0E+00	1.8E+03
257	6.9E+02	4.6E+02	7.8E+02	5.2E+02	2.0E+03	1.3E+03	5.3E+02	8.9E+02	3.8E+03	3.0E+03	0.0E+00	1.8E+03
258	6.9E+02	4.6E+02	7.8E+02	5.2E+02	2.0E+03	1.3E+03	5.3E+02	8.9E+02	3.8E+03	3.0E+03	0.0E+00	1.8E+03
259	6.9E+02	4.6E+02	7.8E+02	5.2E+02	2.0E+03	1.3E+03	5.3E+02	8.9E+02	3.8E+03	3.0E+03	0.0E+00	1.8E+03
260	6.9E+02	4.6E+02	7.8E+02	5.2E+02	2.0E+03	1.3E+03	5.3E+02	8.9E+02	3.8E+03	3.0E+03	0.0E+00	1.8E+03
261	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
262	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
263	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
264	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
265	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
266	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
267	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
268	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
269	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
270	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
271	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
272	1.2E+03	8.2E+02	1.2E+03	7.7E+02	0.0E+00	1.3E+03	7.8E+02	0.0E+00	0.0E+00	1.6E+04	0.0E+00	1.6E+04
273	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
274	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
275	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
276	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
277	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
278	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
279	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
280	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
281	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
282	9.9E+02	6.6E+02	8.0E+02	5.3E+02	0.0E+00	9.3E+02	7.8E+02	0.0E+00	0.0E+00	1.3E+04	0.0E+00	1.4E+04
283	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E+03
284	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E+03
285	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E+03
286	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E+03
287	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E+03
288	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E+03

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
289	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E
290	7.9E+02	5.2E+02	1.1E+03	7.1E+02	0.0E+00	1.4E+03	1.6E+03	0.0E+00	0.0E+00	2.5E+02	0.0E+00	1.6E
291	1.9E+03	1.2E+03	7.5E+02	5.0E+02	5.3E+03	1.8E+03	2.0E+03	2.2E+03	0.0E+00	3.0E+03	2.0E+04	2.0E
292	1.9E+03	1.2E+03	7.5E+02	5.0E+02	5.3E+03	1.8E+03	2.0E+03	2.2E+03	0.0E+00	3.0E+03	2.0E+04	2.0E
293	1.9E+03	1.2E+03	7.5E+02	5.0E+02	5.3E+03	1.8E+03	2.0E+03	2.2E+03	0.0E+00	3.0E+03	2.0E+04	2.0E
294	1.9E+03	1.2E+03	7.5E+02	5.0E+02	5.3E+03	1.8E+03	2.0E+03	2.2E+03	0.0E+00	3.0E+03	2.0E+04	2.0E
295	1.9E+03	1.2E+03	7.5E+02	5.0E+02	5.3E+03	1.8E+03	2.0E+03	2.2E+03	0.0E+00	3.0E+03	2.0E+04	2.0E
296	1.3E+03	8.8E+02	1.1E+03	7.1E+02	8.0E+03	1.7E+03	1.2E+03	3.0E+03	2.0E+04	1.5E+04	2.0E+04	1.5E
297	1.3E+03	8.8E+02	1.1E+03	7.1E+02	8.0E+03	1.7E+03	1.2E+03	3.0E+03	2.0E+04	1.5E+04	2.0E+04	1.5E
298	1.3E+03	8.8E+02	1.1E+03	7.1E+02	8.0E+03	1.7E+03	1.2E+03	3.0E+03	2.0E+04	1.5E+04	2.0E+04	1.5E
299	1.3E+03	8.8E+02	1.1E+03	7.1E+02	8.0E+03	1.7E+03	1.2E+03	3.0E+03	2.0E+04	1.5E+04	2.0E+04	1.5E
300	1.3E+03	8.8E+02	1.1E+03	7.1E+02	8.0E+03	1.7E+03	1.2E+03	3.0E+03	2.0E+04	1.5E+04	2.0E+04	1.5E
301	1.3E+03	8.8E+02	1.1E+03	7.1E+02	8.0E+03	1.7E+03	1.2E+03	3.0E+03	2.0E+04	1.5E+04	2.0E+04	1.5E
302	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
303	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
304	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
305	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
306	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
307	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
308	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
309	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
310	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
311	1.0E+03	6.8E+02	9.0E+02	6.0E+02	9.8E+02	8.3E+02	7.5E+02	1.0E+03	0.0E+00	7.9E+03	0.0E+00	5.8E
312	1.2E+03	8.2E+02	1.4E+03	9.5E+02	3.3E+03	1.6E+03	1.3E+03	1.1E+03	0.0E+00	5.3E+03	6.7E+03	8.7E
313	1.2E+03	8.2E+02	1.4E+03	9.5E+02	3.3E+03	1.6E+03	1.3E+03	1.1E+03	0.0E+00	5.3E+03	6.7E+03	8.7E
314	1.2E+03	8.2E+02	1.4E+03	9.5E+02	3.3E+03	1.6E+03	1.3E+03	1.1E+03	0.0E+00	5.3E+03	6.7E+03	8.7E
315	1.2E+03	8.2E+02	1.4E+03	9.5E+02	3.3E+03	1.6E+03	1.3E+03	1.1E+03	0.0E+00	5.3E+03	6.7E+03	8.7E
316	1.2E+03	8.2E+02	1.4E+03	9.5E+02	3.3E+03	1.6E+03	1.3E+03	1.1E+03	0.0E+00	5.3E+03	6.7E+03	8.7E
317	1.2E+03	8.2E+02	1.4E+03	9.5E+02	3.3E+03	1.6E+03	1.3E+03	1.1E+03	0.0E+00	5.3E+03	6.7E+03	8.7E
318	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
319	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
320	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
321	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
322	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
323	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
324	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
325	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
326	1.7E+03	1.1E+03	1.4E+03	9.6E+02	0.0E+00	1.0E+03	1.0E+03	0.0E+00	2.9E+04	1.0E+04	1.4E+04	1.0E
327	1.5E+03	9.9E+02	1.7E+03	1.1E+03	4.0E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	1.0E+04	6.0E
328	1.5E+03	9.9E+02	1.7E+03	1.1E+03	4.0E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	1.0E+04	6.0E
329	1.5E+03	9.9E+02	1.7E+03	1.1E+03	4.0E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	1.0E+04	6.0E
330	1.5E+03	9.9E+02	1.7E+03	1.1E+03	4.0E+03	1.4E+03	0.0E+00	0.0E+00	0.0E+00	6.5E+03	1.0E+04	6.0E
331	2.0E+03	1.3E+03	1.8E+03	1.2E+03	2.5E+03	2.6E+03	0.0E+00	2.8E+03	5.5E+03	7.6E+03	1.2E+04	7.6E
332	2.0E+03	1.3E+03	1.8E+03	1.2E+03	2.5E+03	2.6E+03	0.0E+00	2.8E+03	5.5E+03	7.6E+03	1.2E+04	7.6E
333	2.0E+03	1.3E+03	1.8E+03	1.2E+03	2.5E+03	2.6E+03	0.0E+00	2.8E+03	5.5E+03	7.6E+03	1.2E+04	7.6E
334	2.0E+03	1.3E+03	1.8E+03	1.2E+03	2.5E+03	2.6E+03	0.0E+00	2.8E+03	5.5E+03	7.6E+03	1.2E+04	7.6E
335	2.0E+03	1.3E+03	1.8E+03	1.2E+03	2.5E+03	2.6E+03	0.0E+00	2.8E+03	5.5E+03	7.6E+03	1.2E+04	7.6E
336	2.0E+03	1.3E+03	1.8E+03	1.2E+03	2.5E+03	2.6E+03	0.0E+00	2.8E+03	5.5E+03	7.6E+03	1.2E+04	7.6E
337	2.0E+03	1.3E+03	1.8E+03	1.2E+03	2.5E+03	2.6E+03	0.0E+00	2.8E+03	5.5E+03	7.6E+03	1.2E+04	7.6E
338	8.0E+02	5.3E+02	8.0E+02	5.4E+02	1.6E+03	6.3E+02	6.3E+02	0.0E+00	6.0E+03	4.5E+03	1.3E+04	0.0E
339	8.0E+02	5.3E+02	8.0E+02	5.4E+02	1.6E+03	6.3E+02	6.3E+02	0.0E+00	6.0E+03	4.5E+03	1.3E+04	0.0E

Table D.12: .-Production yields in rainfed crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
340	8.0E+02	5.3E+02	8.0E+02	5.4E+02	1.6E+03	6.3E+02	6.3E+02	0.0E+00	6.0E+03	4.5E+03	1.3E+04	0.0E+00
341	5.7E+02	3.8E+02	5.7E+02	3.8E+02	1.3E+03	6.6E+02	6.6E+02	0.0E+00	5.3E+03	3.2E+03	0.0E+00	3.2E+03
342	5.7E+02	3.8E+02	5.7E+02	3.8E+02	1.3E+03	6.6E+02	6.6E+02	0.0E+00	5.3E+03	3.2E+03	0.0E+00	3.2E+03
343	5.7E+02	3.8E+02	5.7E+02	3.8E+02	1.3E+03	6.6E+02	6.6E+02	0.0E+00	5.3E+03	3.2E+03	0.0E+00	3.2E+03
344	5.7E+02	3.8E+02	5.7E+02	3.8E+02	1.3E+03	6.6E+02	6.6E+02	0.0E+00	5.3E+03	3.2E+03	0.0E+00	3.2E+03
345	5.7E+02	3.8E+02	5.7E+02	3.8E+02	1.3E+03	6.6E+02	6.6E+02	0.0E+00	5.3E+03	3.2E+03	0.0E+00	3.2E+03

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
1	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
2	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
3	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
4	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
5	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
6	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
7	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
8	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
9	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
10	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
11	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
12	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
13	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
14	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
15	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
16	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
17	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
18	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
19	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
20	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
21	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
22	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
23	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
24	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	3.0E+04	0.0E+00	9.1E+03	0.0E+00
25	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
26	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
27	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
28	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
29	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
30	0.0E+00	0.0E+00	0.0E+00	0.0E+00	7.1E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
31	0.0E+00	0.0E+00	0.0E+00	0.0E+00	7.1E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
32	0.0E+00	0.0E+00	0.0E+00	0.0E+00	7.1E+03	0.0E+00	0.0E+00	0.0E+00	4.3E+04	0.0E+00	9.0E+03	0.0E+00
33	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.1E+03	0.0E+00	0.0E+00	0.0E+00	6.7E+04	0.0E+00	0.0E+00	0.0E+00
34	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.1E+03	0.0E+00	0.0E+00	0.0E+00	6.7E+04	0.0E+00	0.0E+00	0.0E+00
35	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.1E+03	0.0E+00	0.0E+00	0.0E+00	6.7E+04	0.0E+00	0.0E+00	0.0E+00
36	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.1E+03	0.0E+00	0.0E+00	0.0E+00	6.7E+04	0.0E+00	0.0E+00	0.0E+00
37	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
38	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
39	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
40	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
41	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
42	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
43	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
44	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
45	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
46	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
47	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+04	0.0E+00	3.0E+04	1.6E
48	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+04	0.0E+00	3.0E+04	1.6E
49	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+04	0.0E+00	3.0E+04	1.6E
50	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+04	0.0E+00	3.0E+04	1.6E
51	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+04	0.0E+00	3.0E+04	1.6E
52	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+04	0.0E+00	3.0E+04	1.6E
53	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.6E+04	0.0E+00	5.0E+04	3.5E
54	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.6E+04	0.0E+00	5.0E+04	3.5E
55	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.6E+04	0.0E+00	5.0E+04	3.5E
56	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.6E+04	0.0E+00	5.0E+04	3.5E
57	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.6E+04	0.0E+00	5.0E+04	3.5E
58	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.6E+04	0.0E+00	5.0E+04	3.5E
59	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
60	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.6E+03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E
61	3.7E+03	2.5E+03	3.2E+03	2.1E+03	1.2E+04	4.9E+03	4.2E+03	7.5E+03	5.0E+04	2.1E+04	4.2E+04	2.8E
62	3.7E+03	2.5E+03	3.2E+03	2.1E+03	1.2E+04	4.9E+03	4.2E+03	7.5E+03	5.0E+04	2.1E+04	4.2E+04	2.8E
63	3.7E+03	2.5E+03	3.2E+03	2.1E+03	1.2E+04	4.9E+03	4.2E+03	7.5E+03	5.0E+04	2.1E+04	4.2E+04	2.8E
64	3.7E+03	2.5E+03	3.2E+03	2.1E+03	1.2E+04	4.9E+03	4.2E+03	7.5E+03	5.0E+04	2.1E+04	4.2E+04	2.8E
65	3.7E+03	2.5E+03	3.2E+03	2.1E+03	1.2E+04	4.9E+03	4.2E+03	7.5E+03	5.0E+04	2.1E+04	4.2E+04	2.8E
66	3.7E+03	2.5E+03	3.2E+03	2.1E+03	1.2E+04	4.9E+03	4.2E+03	7.5E+03	5.0E+04	2.1E+04	4.2E+04	2.8E
67	3.7E+03	2.5E+03	3.2E+03	2.1E+03	1.2E+04	4.9E+03	4.2E+03	7.5E+03	5.0E+04	2.1E+04	4.2E+04	2.8E
68	3.2E+03	2.1E+03	3.3E+03	2.2E+03	1.2E+04	4.8E+03	4.6E+03	0.0E+00	5.3E+04	2.2E+04	4.7E+04	2.6E
69	3.2E+03	2.1E+03	3.3E+03	2.2E+03	1.2E+04	4.8E+03	4.6E+03	0.0E+00	5.3E+04	2.2E+04	4.7E+04	2.6E
70	3.2E+03	2.1E+03	3.3E+03	2.2E+03	1.2E+04	4.8E+03	4.6E+03	0.0E+00	5.3E+04	2.2E+04	4.7E+04	2.6E
71	3.2E+03	2.1E+03	3.3E+03	2.2E+03	1.2E+04	4.8E+03	4.6E+03	0.0E+00	5.3E+04	2.2E+04	4.7E+04	2.6E
72	3.2E+03	2.1E+03	3.3E+03	2.2E+03	1.2E+04	4.8E+03	4.6E+03	0.0E+00	5.3E+04	2.2E+04	4.7E+04	2.6E
73	3.2E+03	2.1E+03	3.3E+03	2.2E+03	1.2E+04	4.8E+03	4.6E+03	0.0E+00	5.3E+04	2.2E+04	4.7E+04	2.6E
74	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
75	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
76	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
77	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
78	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
79	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
80	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
81	3.0E+03	2.0E+03	3.7E+03	2.4E+03	1.2E+04	3.7E+03	3.6E+03	5.4E+03	6.4E+04	2.0E+04	4.7E+04	2.8E
82	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.2E+04	2.9E+03	3.7E+03	4.7E+03	0.0E+00	1.4E+04	3.3E+04	2.0E
83	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.2E+04	2.9E+03	3.7E+03	4.7E+03	0.0E+00	1.4E+04	3.3E+04	2.0E
84	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.2E+04	2.9E+03	3.7E+03	4.7E+03	0.0E+00	1.4E+04	3.3E+04	2.0E
85	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.2E+04	2.9E+03	3.7E+03	4.7E+03	0.0E+00	1.4E+04	3.3E+04	2.0E
86	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.2E+04	2.9E+03	3.7E+03	4.7E+03	0.0E+00	1.4E+04	3.3E+04	2.0E
87	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.2E+04	2.9E+03	3.7E+03	4.7E+03	0.0E+00	1.4E+04	3.3E+04	2.0E
88	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E
89	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
90	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E+04
91	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E+04
92	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E+04
93	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E+04
94	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E+04
95	2.6E+03	1.8E+03	3.2E+03	2.1E+03	1.1E+04	4.5E+03	4.0E+03	6.0E+03	0.0E+00	1.8E+04	4.8E+04	2.3E+04
96	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
97	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
98	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
99	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
100	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
101	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
102	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
103	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
104	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
105	3.5E+03	2.3E+03	3.5E+03	2.3E+03	1.0E+04	5.4E+03	0.0E+00	0.0E+00	6.6E+04	3.1E+04	6.7E+04	0.0E+00
106	2.6E+03	1.8E+03	2.7E+03	1.8E+03	1.2E+04	2.5E+03	3.5E+03	5.8E+03	5.8E+04	3.0E+04	4.1E+04	2.8E+04
107	2.6E+03	1.8E+03	2.7E+03	1.8E+03	1.2E+04	2.5E+03	3.5E+03	5.8E+03	5.8E+04	3.0E+04	4.1E+04	2.8E+04
108	2.6E+03	1.8E+03	2.7E+03	1.8E+03	1.2E+04	2.5E+03	3.5E+03	5.8E+03	5.8E+04	3.0E+04	4.1E+04	2.8E+04
109	2.6E+03	1.8E+03	2.7E+03	1.8E+03	1.2E+04	2.5E+03	3.5E+03	5.8E+03	5.8E+04	3.0E+04	4.1E+04	2.8E+04
110	2.6E+03	1.8E+03	2.7E+03	1.8E+03	1.2E+04	2.5E+03	3.5E+03	5.8E+03	5.8E+04	3.0E+04	4.1E+04	2.8E+04
111	2.6E+03	1.8E+03	2.7E+03	1.8E+03	1.2E+04	2.5E+03	3.5E+03	5.8E+03	5.8E+04	3.0E+04	4.1E+04	2.8E+04
112	2.6E+03	1.8E+03	2.7E+03	1.8E+03	1.2E+04	2.5E+03	3.5E+03	5.8E+03	5.8E+04	3.0E+04	4.1E+04	2.8E+04
113	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
114	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
115	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
116	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
117	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
118	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
119	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
120	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
121	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
122	2.5E+03	1.7E+03	2.5E+03	1.7E+03	8.0E+03	5.0E+03	5.0E+03	6.7E+03	5.8E+04	2.5E+04	6.2E+04	0.0E+00
123	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
124	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
125	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
126	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
127	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
128	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
129	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
130	1.9E+03	1.3E+03	1.7E+03	1.1E+03	9.0E+03	2.0E+03	0.0E+00	2.5E+03	4.0E+04	1.6E+04	4.5E+04	0.0E+00
131	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+03	0.0E+00	0.0E+00	0.0E+00	4.5E+04	0.0E+00	4.7E+04	0.0E+00
132	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+03	0.0E+00	0.0E+00	0.0E+00	4.5E+04	0.0E+00	4.7E+04	0.0E+00
133	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.5E+03	0.0E+00	0.0E+00	0.0E+00	4.5E+04	0.0E+00	4.7E+04	0.0E+00
134	2.2E+03	1.5E+03	2.1E+03	1.4E+03	1.2E+04	1.1E+03	0.0E+00	0.0E+00	7.0E+04	2.1E+04	6.1E+04	2.4E+04
135	2.2E+03	1.5E+03	2.1E+03	1.4E+03	1.2E+04	1.1E+03	0.0E+00	0.0E+00	7.0E+04	2.1E+04	6.1E+04	2.4E+04
136	2.2E+03	1.5E+03	2.1E+03	1.4E+03	1.2E+04	1.1E+03	0.0E+00	0.0E+00	7.0E+04	2.1E+04	6.1E+04	2.4E+04
137	2.2E+03	1.5E+03	2.1E+03	1.4E+03	1.2E+04	1.1E+03	0.0E+00	0.0E+00	7.0E+04	2.1E+04	6.1E+04	2.4E+04
138	2.2E+03	1.5E+03	2.1E+03	1.4E+03	1.2E+04	1.1E+03	0.0E+00	0.0E+00	7.0E+04	2.1E+04	6.1E+04	2.4E+04
139	2.2E+03	1.5E+03	2.1E+03	1.4E+03	1.2E+04	1.1E+03	0.0E+00	0.0E+00	7.0E+04	2.1E+04	6.1E+04	2.4E+04
140	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E+04

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
141	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E
142	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E
143	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E
144	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E
145	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E
146	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E
147	3.4E+03	2.3E+03	3.1E+03	2.0E+03	1.5E+04	4.4E+03	4.3E+03	0.0E+00	5.5E+04	0.0E+00	5.5E+04	2.5E
148	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
149	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
150	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
151	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
152	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
153	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
154	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
155	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
156	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
157	3.7E+03	2.5E+03	3.1E+03	2.1E+03	1.2E+04	3.3E+03	3.0E+03	8.0E+03	7.0E+04	1.8E+04	5.2E+04	1.8E
158	3.2E+03	2.2E+03	2.9E+03	1.9E+03	1.2E+04	4.8E+03	4.0E+03	7.5E+03	5.6E+04	1.2E+04	5.0E+04	1.8E
159	3.2E+03	2.2E+03	2.9E+03	1.9E+03	1.2E+04	4.8E+03	4.0E+03	7.5E+03	5.6E+04	1.2E+04	5.0E+04	1.8E
160	3.2E+03	2.2E+03	2.9E+03	1.9E+03	1.2E+04	4.8E+03	4.0E+03	7.5E+03	5.6E+04	1.2E+04	5.0E+04	1.8E
161	3.2E+03	2.2E+03	2.9E+03	1.9E+03	1.2E+04	4.8E+03	4.0E+03	7.5E+03	5.6E+04	1.2E+04	5.0E+04	1.8E
162	3.2E+03	2.2E+03	2.9E+03	1.9E+03	1.2E+04	4.8E+03	4.0E+03	7.5E+03	5.6E+04	1.2E+04	5.0E+04	1.8E
163	3.2E+03	2.2E+03	2.9E+03	1.9E+03	1.2E+04	4.8E+03	4.0E+03	7.5E+03	5.6E+04	1.2E+04	5.0E+04	1.8E
164	3.2E+03	2.2E+03	2.9E+03	1.9E+03	1.2E+04	4.8E+03	4.0E+03	7.5E+03	5.6E+04	1.2E+04	5.0E+04	1.8E
165	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
166	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
167	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
168	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
169	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
170	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
171	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
172	2.4E+03	1.6E+03	2.6E+03	1.7E+03	1.3E+04	3.4E+03	0.0E+00	7.0E+03	5.0E+04	1.5E+04	4.5E+04	1.2E
173	2.1E+03	1.4E+03	2.1E+03	1.4E+03	1.1E+04	2.5E+03	2.8E+03	4.0E+03	5.5E+04	3.0E+04	5.4E+04	3.0E
174	2.1E+03	1.4E+03	2.1E+03	1.4E+03	1.1E+04	2.5E+03	2.8E+03	4.0E+03	5.5E+04	3.0E+04	5.4E+04	3.0E
175	2.1E+03	1.4E+03	2.1E+03	1.4E+03	1.1E+04	2.5E+03	2.8E+03	4.0E+03	5.5E+04	3.0E+04	5.4E+04	3.0E
176	3.0E+03	2.0E+03	2.8E+03	1.9E+03	1.2E+04	3.0E+03	4.1E+03	8.5E+03	0.0E+00	0.0E+00	3.8E+04	2.3E
177	3.0E+03	2.0E+03	2.8E+03	1.9E+03	1.2E+04	3.0E+03	4.1E+03	8.5E+03	0.0E+00	0.0E+00	3.8E+04	2.3E
178	3.0E+03	2.0E+03	2.8E+03	1.9E+03	1.2E+04	3.0E+03	4.1E+03	8.5E+03	0.0E+00	0.0E+00	3.8E+04	2.3E
179	3.0E+03	2.0E+03	2.8E+03	1.9E+03	1.2E+04	3.0E+03	4.1E+03	8.5E+03	0.0E+00	0.0E+00	3.8E+04	2.3E
180	3.0E+03	2.0E+03	2.8E+03	1.9E+03	1.2E+04	3.0E+03	4.1E+03	8.5E+03	0.0E+00	0.0E+00	3.8E+04	2.3E
181	3.0E+03	2.0E+03	2.8E+03	1.9E+03	1.2E+04	3.0E+03	4.1E+03	8.5E+03	0.0E+00	0.0E+00	3.8E+04	2.3E
182	3.0E+03	2.0E+03	2.8E+03	1.9E+03	1.2E+04	3.0E+03	4.1E+03	8.5E+03	0.0E+00	0.0E+00	3.8E+04	2.3E
183	2.3E+03	1.6E+03	2.7E+03	1.8E+03	1.3E+04	0.0E+00	0.0E+00	0.0E+00	7.0E+04	0.0E+00	6.0E+04	0.0E
184	2.3E+03	1.6E+03	2.7E+03	1.8E+03	1.3E+04	0.0E+00	0.0E+00	0.0E+00	7.0E+04	0.0E+00	6.0E+04	0.0E
185	2.3E+03	1.6E+03	2.7E+03	1.8E+03	1.3E+04	0.0E+00	0.0E+00	0.0E+00	7.0E+04	0.0E+00	6.0E+04	0.0E
186	2.3E+03	1.6E+03	2.7E+03	1.8E+03	1.3E+04	0.0E+00	0.0E+00	0.0E+00	7.0E+04	0.0E+00	6.0E+04	0.0E
187	2.8E+03	1.9E+03	2.8E+03	1.8E+03	1.4E+04	2.8E+03	3.5E+03	0.0E+00	7.0E+04	0.0E+00	5.5E+04	3.0E
188	2.8E+03	1.9E+03	2.8E+03	1.8E+03	1.4E+04	2.8E+03	3.5E+03	0.0E+00	7.0E+04	0.0E+00	5.5E+04	3.0E
189	2.8E+03	1.9E+03	2.8E+03	1.8E+03	1.4E+04	2.8E+03	3.5E+03	0.0E+00	7.0E+04	0.0E+00	5.5E+04	3.0E
190	2.8E+03	1.9E+03	2.8E+03	1.8E+03	1.4E+04	2.8E+03	3.5E+03	0.0E+00	7.0E+04	0.0E+00	5.5E+04	3.0E
191	2.8E+03	1.9E+03	2.8E+03	1.8E+03	1.4E+04	2.8E+03	3.5E+03	0.0E+00	7.0E+04	0.0E+00	5.5E+04	3.0E

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
192	2.8E+03	1.9E+03	2.8E+03	1.8E+03	1.4E+04	2.8E+03	3.5E+03	0.0E+00	7.0E+04	0.0E+00	5.5E+04	3.0E+04
193	2.5E+03	1.7E+03	2.5E+03	1.7E+03	1.1E+04	3.3E+03	3.1E+03	5.0E+03	5.5E+04	2.6E+04	6.3E+04	0.0E+00
194	2.5E+03	1.7E+03	2.5E+03	1.7E+03	1.1E+04	3.3E+03	3.1E+03	5.0E+03	5.5E+04	2.6E+04	6.3E+04	0.0E+00
195	2.5E+03	1.7E+03	2.5E+03	1.7E+03	1.1E+04	3.3E+03	3.1E+03	5.0E+03	5.5E+04	2.6E+04	6.3E+04	0.0E+00
196	2.5E+03	1.7E+03	2.5E+03	1.7E+03	1.1E+04	3.3E+03	3.1E+03	5.0E+03	5.5E+04	2.6E+04	6.3E+04	0.0E+00
197	2.5E+03	1.7E+03	2.5E+03	1.7E+03	1.1E+04	3.3E+03	3.1E+03	5.0E+03	5.5E+04	2.6E+04	6.3E+04	0.0E+00
198	2.5E+03	1.7E+03	2.5E+03	1.7E+03	1.1E+04	3.3E+03	3.1E+03	5.0E+03	5.5E+04	2.6E+04	6.3E+04	0.0E+00
199	4.5E+03	3.0E+03	4.0E+03	2.7E+03	1.5E+04	5.5E+03	4.6E+03	6.0E+03	6.0E+04	2.5E+04	6.8E+04	1.3E+04
200	4.5E+03	3.0E+03	4.0E+03	2.7E+03	1.5E+04	5.5E+03	4.6E+03	6.0E+03	6.0E+04	2.5E+04	6.8E+04	1.3E+04
201	4.5E+03	3.0E+03	4.0E+03	2.7E+03	1.5E+04	5.5E+03	4.6E+03	6.0E+03	6.0E+04	2.5E+04	6.8E+04	1.3E+04
202	4.5E+03	3.0E+03	4.0E+03	2.7E+03	1.5E+04	5.5E+03	4.6E+03	6.0E+03	6.0E+04	2.5E+04	6.8E+04	1.3E+04
203	4.5E+03	3.0E+03	4.0E+03	2.7E+03	1.5E+04	5.5E+03	4.6E+03	6.0E+03	6.0E+04	2.5E+04	6.8E+04	1.3E+04
204	4.5E+03	3.0E+03	4.0E+03	2.7E+03	1.5E+04	5.5E+03	4.6E+03	6.0E+03	6.0E+04	2.5E+04	6.8E+04	1.3E+04
205	4.5E+03	3.0E+03	4.0E+03	2.7E+03	1.5E+04	5.5E+03	4.6E+03	6.0E+03	6.0E+04	2.5E+04	6.8E+04	1.3E+04
206	2.0E+03	1.4E+03	2.0E+03	1.4E+03	1.2E+04	3.0E+03	2.8E+03	4.9E+03	4.5E+04	0.0E+00	5.4E+04	3.0E+04
207	2.0E+03	1.4E+03	2.0E+03	1.4E+03	1.2E+04	3.0E+03	2.8E+03	4.9E+03	4.5E+04	0.0E+00	5.4E+04	3.0E+04
208	2.0E+03	1.4E+03	2.0E+03	1.4E+03	1.2E+04	3.0E+03	2.8E+03	4.9E+03	4.5E+04	0.0E+00	5.4E+04	3.0E+04
209	2.0E+03	1.4E+03	2.0E+03	1.4E+03	1.2E+04	3.0E+03	2.8E+03	4.9E+03	4.5E+04	0.0E+00	5.4E+04	3.0E+04
210	2.0E+03	1.4E+03	2.0E+03	1.4E+03	1.2E+04	3.0E+03	2.8E+03	4.9E+03	4.5E+04	0.0E+00	5.4E+04	3.0E+04
211	2.0E+03	1.4E+03	2.0E+03	1.4E+03	1.2E+04	3.0E+03	2.8E+03	4.9E+03	4.5E+04	0.0E+00	5.4E+04	3.0E+04
212	3.0E+03	2.0E+03	3.0E+03	2.0E+03	1.2E+04	4.3E+03	4.2E+03	3.8E+03	0.0E+00	1.6E+04	5.8E+04	6.0E+03
213	3.0E+03	2.0E+03	3.0E+03	2.0E+03	1.2E+04	4.3E+03	4.2E+03	3.8E+03	0.0E+00	1.6E+04	5.8E+04	6.0E+03
214	3.0E+03	2.0E+03	3.0E+03	2.0E+03	1.2E+04	4.3E+03	4.2E+03	3.8E+03	0.0E+00	1.6E+04	5.8E+04	6.0E+03
215	3.0E+03	2.0E+03	3.0E+03	2.0E+03	1.2E+04	4.3E+03	4.2E+03	3.8E+03	0.0E+00	1.6E+04	5.8E+04	6.0E+03
216	3.0E+03	2.0E+03	3.0E+03	2.0E+03	1.2E+04	4.3E+03	4.2E+03	3.8E+03	0.0E+00	1.6E+04	5.8E+04	6.0E+03
217	3.0E+03	2.0E+03	3.0E+03	2.0E+03	1.2E+04	4.3E+03	4.2E+03	3.8E+03	0.0E+00	1.6E+04	5.8E+04	6.0E+03
218	3.0E+03	2.0E+03	3.0E+03	2.0E+03	1.2E+04	4.3E+03	4.2E+03	3.8E+03	0.0E+00	1.6E+04	5.8E+04	6.0E+03
219	3.0E+03	2.0E+03	2.7E+03	1.8E+03	1.2E+04	3.5E+03	3.5E+03	2.0E+03	0.0E+00	9.0E+03	5.0E+04	0.0E+00
220	3.0E+03	2.0E+03	2.7E+03	1.8E+03	1.2E+04	3.5E+03	3.5E+03	2.0E+03	0.0E+00	9.0E+03	5.0E+04	0.0E+00
221	3.0E+03	2.0E+03	2.7E+03	1.8E+03	1.2E+04	3.5E+03	3.5E+03	2.0E+03	0.0E+00	9.0E+03	5.0E+04	0.0E+00
222	3.0E+03	2.0E+03	2.7E+03	1.8E+03	1.2E+04	3.5E+03	3.5E+03	2.0E+03	0.0E+00	9.0E+03	5.0E+04	0.0E+00
223	3.0E+03	2.0E+03	2.7E+03	1.8E+03	1.2E+04	3.5E+03	3.5E+03	2.0E+03	0.0E+00	9.0E+03	5.0E+04	0.0E+00
224	2.9E+03	2.0E+03	3.0E+03	2.0E+03	1.1E+04	4.0E+03	3.4E+03	5.0E+03	5.5E+04	2.3E+04	7.3E+04	3.4E+04
225	2.9E+03	2.0E+03	3.0E+03	2.0E+03	1.1E+04	4.0E+03	3.4E+03	5.0E+03	5.5E+04	2.3E+04	7.3E+04	3.4E+04
226	2.9E+03	2.0E+03	3.0E+03	2.0E+03	1.1E+04	4.0E+03	3.4E+03	5.0E+03	5.5E+04	2.3E+04	7.3E+04	3.4E+04
227	2.9E+03	2.0E+03	3.0E+03	2.0E+03	1.1E+04	4.0E+03	3.4E+03	5.0E+03	5.5E+04	2.3E+04	7.3E+04	3.4E+04
228	2.9E+03	2.0E+03	3.0E+03	2.0E+03	1.1E+04	4.0E+03	3.4E+03	5.0E+03	5.5E+04	2.3E+04	7.3E+04	3.4E+04
229	2.9E+03	2.0E+03	3.0E+03	2.0E+03	1.1E+04	4.0E+03	3.4E+03	5.0E+03	5.5E+04	2.3E+04	7.3E+04	3.4E+04
230	2.9E+03	2.0E+03	3.0E+03	2.0E+03	1.1E+04	4.0E+03	3.4E+03	5.0E+03	5.5E+04	2.3E+04	7.3E+04	3.4E+04
231	2.4E+03	1.6E+03	2.4E+03	1.6E+03	1.1E+04	3.2E+03	1.5E+03	6.0E+03	3.0E+04	2.1E+04	6.5E+04	2.4E+04
232	2.4E+03	1.6E+03	2.4E+03	1.6E+03	1.1E+04	3.2E+03	1.5E+03	6.0E+03	3.0E+04	2.1E+04	6.5E+04	2.4E+04
233	2.4E+03	1.6E+03	2.4E+03	1.6E+03	1.1E+04	3.2E+03	1.5E+03	6.0E+03	3.0E+04	2.1E+04	6.5E+04	2.4E+04
234	2.4E+03	1.6E+03	2.4E+03	1.6E+03	1.1E+04	3.2E+03	1.5E+03	6.0E+03	3.0E+04	2.1E+04	6.5E+04	2.4E+04
235	2.4E+03	1.6E+03	2.4E+03	1.6E+03	1.1E+04	3.2E+03	1.5E+03	6.0E+03	3.0E+04	2.1E+04	6.5E+04	2.4E+04
236	2.6E+03	1.7E+03	2.1E+03	1.4E+03	5.5E+03	2.8E+03	2.3E+03	5.4E+03	1.9E+04	1.1E+04	4.5E+04	2.0E+04
237	2.6E+03	1.7E+03	2.1E+03	1.4E+03	5.5E+03	2.8E+03	2.3E+03	5.4E+03	1.9E+04	1.1E+04	4.5E+04	2.0E+04
238	2.6E+03	1.7E+03	2.1E+03	1.4E+03	5.5E+03	2.8E+03	2.3E+03	5.4E+03	1.9E+04	1.1E+04	4.5E+04	2.0E+04
239	2.6E+03	1.7E+03	2.1E+03	1.4E+03	5.5E+03	2.8E+03	2.3E+03	5.4E+03	1.9E+04	1.1E+04	4.5E+04	2.0E+04
240	2.6E+03	1.7E+03	2.1E+03	1.4E+03	5.5E+03	2.8E+03	2.3E+03	5.4E+03	1.9E+04	1.1E+04	4.5E+04	2.0E+04
241	2.6E+03	1.7E+03	2.1E+03	1.4E+03	5.5E+03	2.8E+03	2.3E+03	5.4E+03	1.9E+04	1.1E+04	4.5E+04	2.0E+04
242	2.6E+03	1.7E+03	2.1E+03	1.4E+03	5.5E+03	2.8E+03	2.3E+03	5.4E+03	1.9E+04	1.1E+04	4.5E+04	2.0E+04

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
243	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
244	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
245	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
246	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
247	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
248	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
249	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
250	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
251	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
252	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
253	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
254	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
255	2.2E+03	1.5E+03	2.3E+03	1.5E+03	1.5E+04	3.6E+03	0.0E+00	0.0E+00	1.9E+04	0.0E+00	1.5E+04	1.0E
256	2.8E+03	1.8E+03	1.8E+03	1.2E+03	1.1E+04	3.4E+03	2.2E+03	7.2E+03	1.9E+04	1.3E+04	5.1E+04	1.8E
257	2.8E+03	1.8E+03	1.8E+03	1.2E+03	1.1E+04	3.4E+03	2.2E+03	7.2E+03	1.9E+04	1.3E+04	5.1E+04	1.8E
258	2.8E+03	1.8E+03	1.8E+03	1.2E+03	1.1E+04	3.4E+03	2.2E+03	7.2E+03	1.9E+04	1.3E+04	5.1E+04	1.8E
259	2.8E+03	1.8E+03	1.8E+03	1.2E+03	1.1E+04	3.4E+03	2.2E+03	7.2E+03	1.9E+04	1.3E+04	5.1E+04	1.8E
260	2.8E+03	1.8E+03	1.8E+03	1.2E+03	1.1E+04	3.4E+03	2.2E+03	7.2E+03	1.9E+04	1.3E+04	5.1E+04	1.8E
261	2.8E+03	1.8E+03	1.8E+03	1.2E+03	1.1E+04	3.4E+03	2.2E+03	7.2E+03	1.9E+04	1.3E+04	5.1E+04	1.8E
262	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
263	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
264	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
265	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
266	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
267	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
268	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
269	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
270	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
271	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
272	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
273	1.6E+03	1.1E+03	1.5E+03	1.0E+03	1.4E+04	0.0E+00	0.0E+00	0.0E+00	6.8E+04	0.0E+00	4.2E+04	0.0E
274	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
275	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
276	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
277	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
278	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
279	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
280	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
281	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
282	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
283	1.4E+03	9.1E+02	1.2E+03	8.3E+02	1.5E+04	0.0E+00	0.0E+00	2.3E+03	6.8E+04	0.0E+00	3.8E+04	0.0E
284	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
285	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
286	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
287	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
288	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
289	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
290	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
291	1.9E+03	1.3E+03	1.6E+03	1.1E+03	4.2E+03	2.5E+03	2.7E+03	3.0E+03	1.2E+04	4.2E+03	5.7E+04	1.2E
292	2.3E+03	1.5E+03	1.8E+03	1.2E+03	1.2E+04	2.0E+03	0.0E+00	3.1E+03	1.5E+04	8.0E+03	4.0E+04	0.0E
293	2.3E+03	1.5E+03	1.8E+03	1.2E+03	1.2E+04	2.0E+03	0.0E+00	3.1E+03	1.5E+04	8.0E+03	4.0E+04	0.0E

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Vecth
294	2.3E+03	1.5E+03	1.8E+03	1.2E+03	1.2E+04	2.0E+03	0.0E+00	3.1E+03	1.5E+04	8.0E+03	4.0E+04	0.0E+00
295	2.3E+03	1.5E+03	1.8E+03	1.2E+03	1.2E+04	2.0E+03	0.0E+00	3.1E+03	1.5E+04	8.0E+03	4.0E+04	0.0E+00
296	2.3E+03	1.5E+03	1.8E+03	1.2E+03	1.2E+04	2.0E+03	0.0E+00	3.1E+03	1.5E+04	8.0E+03	4.0E+04	0.0E+00
297	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.3E+04	3.2E+03	1.2E+03	7.0E+03	5.0E+04	2.5E+04	6.5E+04	3.0E+04
298	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.3E+04	3.2E+03	1.2E+03	7.0E+03	5.0E+04	2.5E+04	6.5E+04	3.0E+04
299	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.3E+04	3.2E+03	1.2E+03	7.0E+03	5.0E+04	2.5E+04	6.5E+04	3.0E+04
300	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.3E+04	3.2E+03	1.2E+03	7.0E+03	5.0E+04	2.5E+04	6.5E+04	3.0E+04
301	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.3E+04	3.2E+03	1.2E+03	7.0E+03	5.0E+04	2.5E+04	6.5E+04	3.0E+04
302	2.8E+03	1.8E+03	2.3E+03	1.6E+03	1.3E+04	3.2E+03	1.2E+03	7.0E+03	5.0E+04	2.5E+04	6.5E+04	3.0E+04
303	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
304	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
305	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
306	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
307	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
308	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
309	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
310	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
311	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
312	1.9E+03	1.3E+03	1.4E+03	9.5E+02	1.1E+04	3.0E+03	2.2E+03	5.0E+03	3.7E+04	2.7E+04	5.2E+04	1.5E+04
313	1.9E+03	1.2E+03	1.7E+03	1.1E+03	1.0E+04	2.6E+03	0.0E+00	0.0E+00	5.4E+04	2.2E+04	1.7E+04	1.5E+04
314	1.9E+03	1.2E+03	1.7E+03	1.1E+03	1.0E+04	2.6E+03	0.0E+00	0.0E+00	5.4E+04	2.2E+04	1.7E+04	1.5E+04
315	1.9E+03	1.2E+03	1.7E+03	1.1E+03	1.0E+04	2.6E+03	0.0E+00	0.0E+00	5.4E+04	2.2E+04	1.7E+04	1.5E+04
316	1.9E+03	1.2E+03	1.7E+03	1.1E+03	1.0E+04	2.6E+03	0.0E+00	0.0E+00	5.4E+04	2.2E+04	1.7E+04	1.5E+04
317	1.9E+03	1.2E+03	1.7E+03	1.1E+03	1.0E+04	2.6E+03	0.0E+00	0.0E+00	5.4E+04	2.2E+04	1.7E+04	1.5E+04
318	1.9E+03	1.2E+03	1.7E+03	1.1E+03	1.0E+04	2.6E+03	0.0E+00	0.0E+00	5.4E+04	2.2E+04	1.7E+04	1.5E+04
319	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
320	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
321	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
322	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
323	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
324	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
325	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
326	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
327	2.1E+03	1.4E+03	1.8E+03	1.2E+03	1.4E+04	1.5E+03	0.0E+00	3.1E+03	4.3E+04	2.0E+04	5.0E+04	2.2E+04
328	2.5E+03	1.6E+03	2.4E+03	1.6E+03	9.5E+03	3.5E+03	0.0E+00	7.5E+03	0.0E+00	1.2E+04	3.0E+04	1.2E+04
329	2.5E+03	1.6E+03	2.4E+03	1.6E+03	9.5E+03	3.5E+03	0.0E+00	7.5E+03	0.0E+00	1.2E+04	3.0E+04	1.2E+04
330	2.5E+03	1.6E+03	2.4E+03	1.6E+03	9.5E+03	3.5E+03	0.0E+00	7.5E+03	0.0E+00	1.2E+04	3.0E+04	1.2E+04
331	2.5E+03	1.6E+03	2.4E+03	1.6E+03	9.5E+03	3.5E+03	0.0E+00	7.5E+03	0.0E+00	1.2E+04	3.0E+04	1.2E+04
332	2.8E+03	1.9E+03	2.2E+03	1.4E+03	1.4E+04	3.2E+03	0.0E+00	6.8E+03	4.0E+04	2.0E+04	4.8E+04	2.0E+04
333	2.8E+03	1.9E+03	2.2E+03	1.4E+03	1.4E+04	3.2E+03	0.0E+00	6.8E+03	4.0E+04	2.0E+04	4.8E+04	2.0E+04
334	2.8E+03	1.9E+03	2.2E+03	1.4E+03	1.4E+04	3.2E+03	0.0E+00	6.8E+03	4.0E+04	2.0E+04	4.8E+04	2.0E+04
335	2.8E+03	1.9E+03	2.2E+03	1.4E+03	1.4E+04	3.2E+03	0.0E+00	6.8E+03	4.0E+04	2.0E+04	4.8E+04	2.0E+04
336	2.8E+03	1.9E+03	2.2E+03	1.4E+03	1.4E+04	3.2E+03	0.0E+00	6.8E+03	4.0E+04	2.0E+04	4.8E+04	2.0E+04
337	2.8E+03	1.9E+03	2.2E+03	1.4E+03	1.4E+04	3.2E+03	0.0E+00	6.8E+03	4.0E+04	2.0E+04	4.8E+04	2.0E+04
338	2.8E+03	1.9E+03	2.2E+03	1.4E+03	1.4E+04	3.2E+03	0.0E+00	6.8E+03	4.0E+04	2.0E+04	4.8E+04	2.0E+04
339	1.3E+03	8.8E+02	1.9E+03	1.3E+03	3.5E+03	3.5E+03	0.0E+00	0.0E+00	1.5E+04	1.5E+04	3.7E+04	0.0E+00
340	1.3E+03	8.8E+02	1.9E+03	1.3E+03	3.5E+03	3.5E+03	0.0E+00	0.0E+00	1.5E+04	1.5E+04	3.7E+04	0.0E+00
341	1.3E+03	8.8E+02	1.9E+03	1.3E+03	3.5E+03	3.5E+03	0.0E+00	0.0E+00	1.5E+04	1.5E+04	3.7E+04	0.0E+00
342	9.0E+02	6.0E+02	9.0E+02	6.0E+02	3.0E+03	1.0E+03	0.0E+00	0.0E+00	2.0E+04	1.5E+04	3.4E+04	1.7E+04
343	9.0E+02	6.0E+02	9.0E+02	6.0E+02	3.0E+03	1.0E+03	0.0E+00	0.0E+00	2.0E+04	1.5E+04	3.4E+04	1.7E+04
344	9.0E+02	6.0E+02	9.0E+02	6.0E+02	3.0E+03	1.0E+03	0.0E+00	0.0E+00	2.0E+04	1.5E+04	3.4E+04	1.7E+04

Table D.13: .-Production yields in irrigated crops (kg/ha) (Ministerio de Agricultura pesca y alimentación, 2019b)

Code	Wheat.G	Wheat.S	Barley.G	Barley.S	Corn	Oat	Rye	Sorgo	Corn.St	Barley.St	Alfalfa	Ve
345	9.0E+02	6.0E+02	9.0E+02	6.0E+02	3.0E+03	1.0E+03	0.0E+00	0.0E+00	2.0E+04	1.5E+04	3.4E+04	1.7E

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E

APPENDIX E: SUPPLEMENTARY INFORMATION OF CHAPTER 7

Energetic evaluation of the biodiesel

We can estimate the yield to produce biodiesel from the spent coffee ground using the work of Döhlert et al., 2016. The humidity of the SCG is usually of 60%, is that to say, there are 40kg of solids in 100 kg of SCG. Following the work of Döhlert et al., 2016, the percent of biodiesel that you can obtain is 7.27%. Therefore, we can produce 2.91 Kg of biodiesel per 100kg of wet SCG. However, we have to remove 60 Kg (per 100 kg of wet SCG) before. If this evaporation is carried out in atmospheric pressure, the necessary energy is given by Eq.(E.1):

$$E_v = 60kg \cdot \lambda \left(\frac{kcal}{kg}\right) = 60kg \cdot 538.86\frac{kcal}{kg} = 32331.6kcal \tag{E.1}$$

Where λ is the latent heat of vaporization of water (538.86 kcal/kg) (García & Barreiro, 1982) and the heat of combustion of the biodiesel is 9500 kcal/kg (Alejandro et al., 2015). Whether we use all biodiesel to produce energy, we obtain 27645 kcal. Therefore, the energetic balance is shown by Eq. (E.2):

$$Balance = 27645kcal - 32331kcal = -4698kcal/100kg\, wSCG \tag{E.2}$$

The balance is negative, so the process is energetically infeasible.

Economic evaluation of biodiesel

The price of biodiesel can be found in the annual reports on biofuels in Brazil (Barros, 2019). The price of the biodiesel in June of 2019 was 328€ / t. Considering the performance that was calculated in the previous section, the income of the sale of the produced biodiesel from 100 kg of the wet spent coffee ground is 0.95€. However, to produce 2.91 kg Biodiesel, it is necessary to use 85 kg of spent coffee ground to produce hot air to dry the raw material. The cost of the spent coffee ground is 50€/tn (Brazinha et al., 2015). When we produce hot air, we also produce steam that can be sell. The price of industrial steam 7.1€/tn (Elizondo, 2007). We can generate 340 kg of steam burning the 85kg of spent coffee. The income of the sales of the steam is 2.4€/tn. Therefore, the economic balance is shown by Eq.(E.3):

$$Balance = 2.4€/t + 0.95€/tn - 4.25€/t = -0.9€/t \tag{E.3}$$

This balance is also negative.

Estimation of equipment costs.

Filter costs: Granular filters, nanofilters, and reverse osmosis.

The membrane modules are the same used in the work of Brazinha et al., 2015. Therefore, the same price (300€ / m^2) and the same filtering area per module (2.8 m^2 for the reverse osmosis process and 2.5 m^2 for the nanofiltration process) are used. The capacity of each module can be consulted in Lenntech, 2020 and these values are 2.6 m^3/day for inverse osmosis and 2.8 m^3/day for nanofilter. The cost of the reverse osmosis modules of Process 1 is 61078€ and the modules of nanofiltration of the same process have a cost of 58768€.

The equipment cost simulator (Matches, 2014) is used to estimate the cost of the granular bed filter. It is necessary to calculate the filtering area. The filtering area is calculated using the filtering speed and the inlet flow to the filter. The granular bed filtration speed for fast filters is between 4 m/h and 50 m/h (Lopez et al., 2015). In order to be conservative in estimating costs, the lowest filtering speed is selected. The filtering area is 1.16m^2. Prices need to be updated until 2019 due to the fact that the program has prices of 2014. Eq.(E.4) is used with CEPCI2014 (576.1) and CEPCI2019 (618) that were consulted in Engineering, 2020. The cost of the filter updated to 2019 is 29305€.

$$C\left(kN_{2019}\right) = C\left(k\$_{2014}\right) \cdot \frac{618}{567.3} \cdot \frac{0.915€}{1\$} \tag{E.4}$$

Estimation of the extractor, the bed of Fe_2O_3, and PSA cost.

The cost of PSA is calculated by the cost of the support and the cost of the absorbent material. The cost of the support can be estimated as a cylindrical horizontal vessel. It is necessary to know the volume of the vessel. This volume is determined by the mass of the absorbent necessary to adsorb 95% of the CO_2. 100% of H_2O and NH_3 are also absorbed. The adsorbent mass is calculated with Eq.(E.5).

$$m_{Zeolite} = \frac{1}{q \cdot 0.65} \frac{f c_{CO_2} \cdot 1000}{MW_{(CO_2)}} \eta \cdot \tau \tag{E.5}$$

Where q is the adsorption capacity of the bed and is modelled using the Langmuir isothem (Eq.(E.6)). f_{CO_2} is the flow of the CO_2, MW is the molecular weight of the CO_2, n is the adsorption yield (0.95) and τ is the operation time, that must be below 20 min (Hauchhum & Mahanta, 2014).

$$q = \frac{q_m \cdot K \cdot P_{CO_2}}{1 + K \cdot P_{CO_2}} \tag{E.6}$$

Where q_m and K are calculated by Eqs. (E.7) and (E.8) (Martín-Hernández et al., 2020). T is the operating temperature (25ºC).

$$q_m = \text{-1.82355} \cdot 10^{-02}\ T\,(^{o}C) \ + \ 3.72021 \tag{E.7}$$

$$K = \ 1.63070 \cdot 10^{-03}\ T(^{o}C)^2 - \ 3.68662 \cdot 10^{-01}\ T\,(^{o}C) \ + \ 27.3737 \tag{E.8}$$

Therefore, the volume of the vessel is given by Eq.(E.9) and is 1.63m^3. Where the density of the bed is 40lb/ft^3 (Sigma-Aldrich, 2020).

$$V_{vessel} = \frac{m_{Zeolite}}{p_{bed}} \tag{E.9}$$

The relation between diameter and length should be 3 for a pressure of 4.5 bar (Couper et al., 2005). Therefore, the diameter is 0.83 m and the length is 2.5 m. The pressure is not very high, and the practical minimum thickness can be used. For a diameter of 1 meter, the minimum thickness must be 5 mm (Sinnott, 2005) and for a diameter between 1 and 2 meters, it must be 7 mm (for the case of the extractor). The weight can be calculated as indicated in the equation Eq.(E.10).

$$W = \rho_{steel} \cdot \left(\Pi \cdot \left(\left(\frac{D}{2} + e \right)^2 - \left(\frac{D}{2} \right) \right)^2 \right) \cdot L + \frac{4}{3} \cdot \Pi \cdot \left(\left(\frac{D}{2} + e \right)^3 - \left(\frac{D}{2} \right)^3 \right) \tag{E.10}$$

Where ρ_{steel} is the density of the steel (8000 kg / m^3), D is the diameter and L is the length. The weight is 350Kg. The correlation of Couper et al., 2005 is used to estimate the cost of the PSA tower and is shown by Eq. (E.12)-(E.14), where Fm is the material factor whose value is 1.7. The cost of the PSA vessel is 17797.70€ and the update cost is 25033.71€.

The adsorbent used is Zeolite 4A, which can be used for 5 years. Therefore, it will be necessary to replace it 4 times during the useful life of the plant. The cost of the zeolite considered is $ 5 / kg (Xiao et al., 2013).

Two PSA towers must be used.The total cost of the unit is shown by the Eq.(E.11)

$$CostPSA = (CostVessel + CZeolite \cdot MZeolite \cdot 4) \cdot 2 \tag{E.11}$$

The total cost of the two PSA towers is € 89,000. In the case of the extractor, since it is designed as a cylindrical vertical vessel, Eq. (E.12), (E.15) and (E.16) must be used. Its cost is 88885.35€.

$$C = F_M \cdot C_B \cdot C_A \tag{E.12}$$

$$CB = 1.218 \cdot exp \left[8.571 - 0.2330 \cdot (lnW\,(lb)) + 0.04333 \cdot (lnW\,(lb))^2\right] \tag{E.13}$$

$$CA = 1669 \cdot D(ft)^{0.2029} \tag{E.14}$$

$$CB = 1.218 \cdot exp \left[9.100 - 0.2889\,(lnW) + 0.04576(lnW)^2\right] \tag{E.15}$$

$$CA = 300 \cdot D(ft)^{0.7396} L(ft)^{0.7066} \tag{E.16}$$

The bed of Fe_2O_3 will be modeled following the same methodology as in the PSA unit. To determine its volume, the mass of Fe_2O_3 necessary to eliminate the hydrogen sulfide from the gas stream will be used. Since the amount of hydrogen Sulfide is very small, the necessary amount of Fe_2O_3 is considered for a period of 10 years of operation of the plant. Fe2O3 can remove 2.5 gFe_2O_3 per gH_2S (Siefers, 2010). Therefore, the necessary mass of Fe_2O_3 is given by Eq.(E.17). and it is 1603.5 Kg of Fe_2O_3

$$m_{Fe_2O_3} = \frac{F_{H2S}(kg/year)}{2.5\,kg} 10 \tag{E.17}$$

The volume is calculated by Eq.(E.18). and the value is 2.5 m^3.

$$V_{vessel=}\ \frac{m_{Zeolite}}{p_{lecho}} \tag{E.18}$$

The price of Fe_2O_3 is 1.4 $ / kg (Statista, 2020). Therefore, the final price of the bed of Fe2O3 is calculated by Eq.(E.19). and the value € 33254.

$$Cost_{Desulfurizer} = (Cost_{Vessel} + Cost_{Fe_2O\ 3}) \cdot 2 \tag{E.19}$$

Estimation of the scrubber cost

The equipment cost simulator (Matches, 2014) is used to estimate the cost of the scrubber. Note that it is necessary to update the prices from 2014 using Eq.(E.4). The cost of this equipment in 2019 is 4515€.

Cost of heat exchangers The heat exchange area must be calculated for the estimation of the costs of heat exchangers using the formula shown by Eq.(E.20).

$$Q = A \cdot U \cdot LMTD \tag{E.20}$$

All heat exchangers are partial condensers of steam, so the global energy transfer coefficient (U) is 0.20 kcal/s·m^2·K (Sinnott, 2005). The logarithmic mean temperature difference can be calculated as indicated by Eq.(E.21).

$$LMTD = \frac{t_2 - t_1}{\ln\left(\frac{T_s - t_1}{T_s - t_2}\right)} \tag{E.21}$$

Where t_2(K) is the inlet temperature of the cold stream, t_1(K) is the outlet stream, and T_s(K) is the saturation temperature of the steam. The heat exchanged in IQ_1 is 22.69 kcal / s and in IQ_2 is 50.43 kcal/s (**see Figure 3**). The area is 1.27 m^2 for IQ_1 and 2.88 m^2 for IQ_2. The cost is calculated using the correlation of Couper et al., 2005 given by Eq.(E.22). fm_1 and fp_1 are the material and pressure factor, respectively. The updated cost is 2498€ for IQ_1, € for 2860€ IQ_2.

$$C = 1096 \cdot f_m \cdot f_p \cdot A\left(ft^2\right)^{0.18} \tag{E.22}$$

Dryers

Among the wide variety of dryers available, the spray drier is selected because it is the most recommended dryer in the reference (Couper et al., 2005) to dry pigments and natural extracts. There is a correlation (Couper et al., 2005) that relate to the design cost of spray driers with the evaporation rate. This correlation is showed by Eq.(E.23)

$$C(k\$_{2003}) = 1.218 \cdot F_M \cdot e^{\left(0.8403 + 0.8526 \cdot \left(lnx\left(\frac{lb}{h}\right)\right) - 0.0229 \cdot \left(lnx\left(\frac{lb}{h}\right)\right)^2\right)} \tag{E.23}$$

Where F_M is a material factor whose value for the carbon steel is 0.33 and x is the evaporation rate (2227.8lb/h for the pigment and 540.60lb/h for the natural extract). Therefore, the cost is 170802 $\$_{2003}$ for the drying of the pigment and 80410 $\$_{2003}$ in the case of the extract. It is necessary to update this cost to the current year using the CEPCI value of 2003 (Woods, 2007) that is 402 and Eq.(E.4). Thus, the updated costs are 240246.21 €$_{2020}$ and 113108 €$_{2020}$

Decanter

The decanter is designed as a storage tank. The volume is calculated with Eq.(E.24) but using a residence time of 2 h (Brazinha et al., 2015). This volume is 28.56 m^3 or 7545 gal. The formula used for its cost is the one shown by Eq.(E.25) (Couper et al., 2005). F_M is the material factor and is 0.55 (concrete). The updated cost is 17147.5€.

$$V = \frac{\dot{m}}{p} \cdot t_r \tag{E.24}$$

$$C = 1.218 \cdot F_m \cdot \exp[2.631 + 1.3673 \cdot (\ln V\,(gal)) - 0.06309 \cdot (\ln V\,(gal))^2] \tag{E.25}$$

Boiler

Since the boiler does not have a large capacity, its cost is estimated as a fired heater. Therefore, it is necessary to know the energy produced. The feed to the boiler is 1709kg/h and the heat of combustion of the spend coffee ground is 20Mj / kg. Therefore, the energy generated is 32.43 MBTU / h. The cost of this equipment is estimated using the correlation of Couper et al., 2005 shown by the equation Eq.(E.26), where k is 27.3, f_d is 0 and f_p is 0. The updated cost is 931556€.

$$C = 1.218 \cdot k \cdot (1 + f_d + f_p) \cdot Q(\frac{BTU}{h})^{0.86} \tag{E.26}$$

Digestor

The cost of the digestor can be estimated using its volume. The relation between the size of the reactor and the cost per m^3 can be seen in Table E.1. The volume is calculated using Eq.(E.24), the residence time of 21 days, inlet flow of 45046 t/year, and the density is 1.06 g/cm^3. The volume is 2445.5 m^3. Two reactors of 1225 m^3 are considered. The cost of each reactor is 427200€ and, thus, the total cost is 854400€.

Table E.1: Cost of the digestor (Agency of residues of Cataluña, 2016)

Volume of the reactor(m^3)	**Cost of the reactor per m^3 (€/m^3)**
50	1999.85
200	910.60
800	413.47
1200	356.39

Fixed Capital. It is necessary to calculate the physical plant cost (PPC) from the total purchase cost of major equipment items (PCE) to determine the fixed capital of the plant. A factorial method is used. The installation factors for the equipment considered are shown in Table E.2. In total, the PCE is 4.08M€. In addition to equipment costs, it is necessary to consider the cost of equipment erection, piping, instrumentation, electrical and storages. Thus, the physical cost of the plant is calculated by the Eq.(E.27). The values of these factors are shown in Table E.3.

$$PPC = PCE\left(1 + \sum_i f_i\right) \tag{E.27}$$

The value of PPC is €9.59M. It is necessary to consider 3 more costs to calculate the fixed capital (Design and Engineering, Contractor's fee, Contingency). Its factors are shown in Table E.3 as well. The Eq.(E.27) is used but with the new factors. The fixed capital is 13.43M. To calculate the total investment, it is necessary to consider the working capital, which can be estimated as 5% of the fixed capital. Therefore, the total investment is 14.11M

Operation Cost. The operational cost is constituted by a variable cost and a fixed cost. On the one hand, the variable cost is formed by raw material, miscellaneous, utilities, and power. Raw material, utilities, and power costs can be calculated using the mass and energy balances of the superstructure. The rest of the costs can be estimated as a percentage of other costs. On the other hand, the fixed cost is formed by maintenance, operating labour, plant overheads, laboratory, capital charges, and insurance. It is considered that 0.57 jobs are generated by each million euro invested (Martín, 2016). Thus, 2 jobs are generated. However, this value is insufficient to cover the work shifts, which are 5. 5 workers are used. An online consultant is used (salario, 2020) to determine the workers' annual salary. It is recommended to increase the salary by 50% to consider associated expenses or holidays, shift allowances, national insurance, pension contributions, and any other

Table E.2: Installation factors

Boiler	1.5
Extractor	1.7
Decantator	2.3
Filter	1.4
Dryers	1.6
Digestor	2.3
Scrubber	1.7
PSA	1.7
Heat Exchangers	1.5

Table E.3: Factors of the main costs

Cost	Factor (fi)
Equipment erection	0.45
Piping	0.45
Instrumentation	0.15
Electrical	0.10
Storages	0.20
Design and Engineering	0.25
Contractor's fee	0.05
Contingency	0.10

Table E.4: Variable operation costs

Variable operation cost	Value(k€/year)
Raw Material	1.43
Miscellaneous (10% of the Maintenance cost)	0.07
Utilities	0.11
Power	0.36
Total	1.97

Table E.5: Fixed operation cost

Fixed operation cost	Value (MM€/year)
Maintenance (5% of fixed capital)	0.672
Operating labour	0.077
Plant overheads (50% of operating labour)	0.039
Laboratory (30% of operating labour)	0.023
Capital charges (10% of fixed capital)	1.344
Insurance (1% of fixed capital)	0.134
Total	2.289

overheads (Sinnott, 2005). The updated salary would be 15489€ / year and the operating labor is 77444 €/ year. The rest of the costs are shown in Tables E.4 and E.5. The total cost of operating costs is 4.40M.

Sensitivity analysis

The complete results of the sensitivity study can be consulted in Table E.6. Pnp and Pne are the prices of the natural pigment and the natural extract, respectively. Dnp and Dne are the percentage sold of natural pigment and natural extract.

Table E.6: Sensitivity analysis for different demands and prices

Scenario	Pnp(€/kg)	Pne(€/kg)	Dnp(%)	Dne(%)	Profit(M€/year)
1	14	35	3	3	598.3642
2	14	50	3	3	687.3232
3	14	70	3	3	805.9353
4	14	35	3	6	805.9353
5	14	50	3	6	983.53
6	14	70	3	6	1221.0774
7	14	35	3	10	1082.69
8	14	50	3	10	1379.23
9	14	70	3	10	1774.6
10	14	35	6	3	1510
11	14	50	6	3	1598.98
12	14	70	6	3	1717.6
13	14	35	6	6	1717.6
14	14	50	6	6	1895.5124
15	14	70	6	6	2132
16	14	35	6	10	1994.435
17	14	50	6	10	2291
18	14	70	6	10	2686.3887
19	14	35	10	3	2725.5687
20	14	50	10	3	2814
21	14	70	10	3	2933
22	14	35	10	6	2933
23	14	50	10	6	3111
24	14	70	10	6	3348
25	14	35	10	10	3209
26	14	50	10	10	3506
27	14	70	10	10	3901
28	20	35	3	3	989
29	20	50	3	3	1078
30	20	70	3	3	1196.46
31	20	35	3	6	1196.46
32	20	50	3	6	1374.5644
33	20	70	3	6	1611.7885
34	20	35	3	10	1473.4
35	20	50	3	10	1769.9378

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F

APPENDIX F: SUPPLEMENTARY INFORMATION OF CHAPTER 8

F.1 FRAMEWORK DEVELOPMENT

The following sections present the modeling of the proposed processes to treat the grape pomace, that is, combustion, gasification, anaerobic digestion, pyrolisis, oil extractions and polyphenols production.

F.1.1 *Model of the combustion*

From the empirical formula of grape pomace ($C_1H_{1.363}N_{0.033}$ $O_{0.476}$), which can be determined from its elemental composition (see Table F.1) is possible to estimate the mass and energy balances of the combustion process.

The mass balance are carried out from the balance to atoms of carbon (Eq.(F.1)), oxygen (Eq.(F.2)), hydrogen (Eq.(F.3)), and nitrogen (Eq.(F.4)). In addition, Eq.(F.5) and Eq.(F.6) are added to consider that the nitrogen in the air does not react and that a 150% excess of oxygen is considered. This excess air is used to ensure complete oxidation of the compounds used in the reaction and to avoid very high combustor temperatures.

$$z \cdot Nin_{RM} = Nout_{CO_2} \tag{F.1}$$

$$\begin{aligned} x \cdot Nin_{RM} + 2 \cdot Nin_{O_2} + Nin_{H_2O} = 2 \cdot Nout_{O_2} + \\ Nout_{H_2O} + 2 \cdot Nout_{CO_2} + 2 \cdot Nout_{NO_2} \end{aligned} \tag{F.2}$$

$$y \cdot Nin_{RM} + 2 \cdot Nin_{H_2O} = 2 \cdot Nout_{H_2O} \tag{F.3}$$

$$c \cdot Nin_{RM} = Nout_{NO_2} \tag{F.4}$$

$$Nin_{N2} = Nout_{N2} \tag{F.5}$$

$$Nin_{O2} \cdot 0.4 = NoutO2 \tag{F.6}$$

Table F.1: Ultimate analysis (wt%) of grape pomace (Ateş et al., 2019).

Component	wt%
C	47.27
H	5.88
N	1.77
O	45.08

Where z, x, y, c are the coefficients associated with carbon, oxygen, hydrogen and nitrogen respectively. The heat released in the combustion reaction is calculated from the enthalpy of formation (see Table F.2) through Eq.(F.7). Nin_j and Nout_j are the input and output moles of the combustor of component 'j'.

$$\begin{aligned} Q_{comb} = \sum_j (AHf_j \cdot Nout_j) - \\ \sum_j (AHf_j \cdot Nin_j) \quad \forall j \in \{j = O_2, H_2O, CO_2 \;\; and \;\; NO_2\} \end{aligned} \tag{F.7}$$

The combustor is designed so that approximately 40% of the heat is used to produce steam and 60% of the heat is used to heat the flue gas. The final flue gas temperature is calculated by Eqs.(F.8)-(F.11) while the amount of steam generated is estimated by Eq.(F.12).

$$\begin{aligned} \sum_j (AHf_j \cdot 0.6 \cdot Nout_j + Cpout_j \cdot Nout_j) = \\ \sum_j (AHf_j \cdot 0.6 \cdot Nin_j + Cin_j \cdot Nin_j) \end{aligned} \tag{F.8}$$

$$\begin{aligned} Cpout_j = A_j(Tout - Tref) + B_j \cdot \frac{1}{2} \cdot (Tout - Tref)^2 + \\ C_j \cdot \frac{1}{3} \cdot (Tout - Tref)^3 + D_j \cdot \frac{1}{4} \cdot (Tout - Tref)^4 \end{aligned} \tag{F.9}$$

$$Cpin_j = A_j(Tin - Tref) + B_j \cdot \frac{1}{2} \cdot (Tin - Tref)^2 + \tag{F.10}$$

$$C_j \cdot \frac{1}{3} \cdot (Tin - Tref)^3 + D_j \cdot \frac{1}{4} \cdot (Tin - Tref)^4 \tag{F.11}$$

$$m_{steam} \cdot \lambda_{H_2O} = \sum_j (AHf_j \cdot 0.4 \cdot Nout_j) - (AHf_j \cdot 0.4 \cdot Nin_j + Cp_j \cdot Nin_j) \tag{F.12}$$

Where Tout and Tin are the inlet and outlet temperatures of the combustor, AHf$_j$ is the enthalpy of formation of each compound 'j' and Cp$_j$ is the heat capacity of each compound 'j'. A$_j$,B$_j$, C$_j$, and D$_j$ are empirical coefficient which depend on the chemical properties of each compound (Sinnot, 2005a). These parameters together with the enthalpy of formation can be found in Table F.2.

Table F.2: Enthalpy of formation and parameters to calculate the heat capacity of each compound

	AH(kj/mol)	A	B	C	D
CH_4	-74860	19.521	5.21E-02	1.20E-05	-1.13E-08
O_2	0	28.106	-3.68E-06	1.75E-05	-1.07E-08
CO_2	-393770	19.795	7.34E-02	-5.60E-05	1.72E-08
H_2O	-242000	32.243	1.92E-03	1.06E-05	-3.60E-09
N_2	0	31.150	-0.0136	2.68E-05	-1.17E-08
NO_2	33272.8	24.233	48.358E-03	-2.071E-05	29.308E-11

The heat released in combustion is used to feed the hot reservoir of a regenerative Rankine cycle, whose T-S diagram can be seen in Figure F.1.

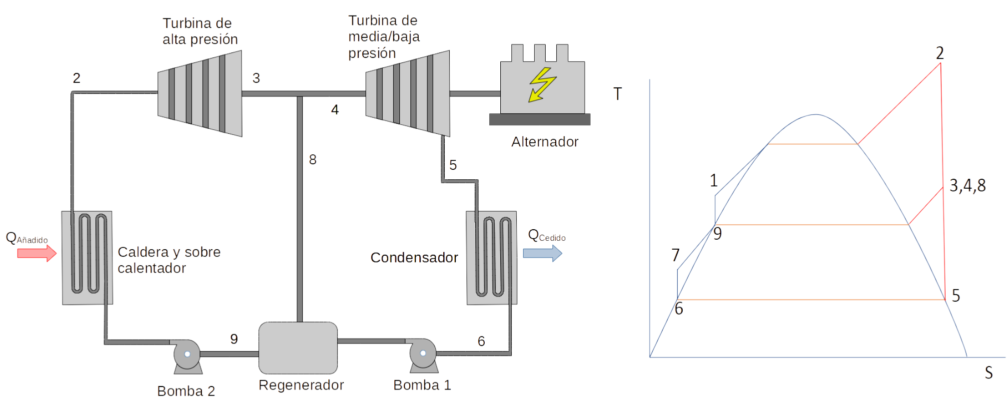

Figure F.1: Regenerative rankine cycle

At the hot reservoir of the cycle, a liquid stream (stream 9) is converted into superheated steam (stream 2). Since the temperature and pressure of stream 2 are set at 100 bar and 555K respectively (León & Martín, 2016), the heat generated in the combustion sets the water mass flow rate of the Ranquine cycle (steam 2).

$$0.4 \cdot Q_{comb} = F2 \cdot (Hwa2 - Hwa1) \tag{F.13}$$

The enthalpy of stream 2 can be calculated from the stream pressure and temperature following Eq. (F.14) (León & Martín, 2016).

$$\begin{aligned} Hwa = {} & (-0.00000000000011619 \cdot P^2 - 0.0000000000087596 \cdot P - \\ & 0.00000000022611)(T)^4 + (0.0000000004298 \cdot P^2 + 0.00000003276 \cdot P \\ & + 0.0000007313) \cdot (T)^3 + (-0.0000005801 \cdot P^2 - 0.000046 \cdot P \\ & - 0.0005009) \cdot (T)^2 + (0.0003383 \cdot P^2 + 0.02947 \cdot P + 2.195) \cdot (T) + \\ & (-0.072042 \cdot P^2 - 7.7877 \cdot P + 2440.8) \end{aligned} \tag{F.14}$$

The entropy also depends on these two variables and can be determined from Eq.(F.15) (León & Martín, 2016).

$$\begin{aligned} Swa = {} & (0.000000000015719 \cdot P + 0.00000000074013) \cdot (T)^3 + \\ & (-0.00000000010074 \cdot P^2 - 0.000000030171 \cdot P - 0.0000028872) \cdot (T)^2 + \\ & (0.000000094914 \cdot P^2 + 0.000029097 \cdot P + 0.0050938) \cdot (T) + \\ & (0.000041223 \cdot P^2 - 0.028841 \cdot P + 5.9537) \end{aligned} \tag{F.15}$$

Since the expansion process in the turbine can be considered isentropic, the temperature in stream 3 can be determined if the pressure of this stream is known. This pressure is fixed at 11 bar (León & Martín, 2016). Since the temperature and pressure of stream 3 are known, the enthalpy can be determined following Eq.(F.14). With this information, the energy generated in the first turbine can be determined by Eq.(F.16).

$$W_{turbine1} = F_2 \cdot (Hwa_3 - Hwa_2) \tag{F.16}$$

After this first turbine, there is a splitter, and therefore, steams 4 and 8 have the same operating conditions (same entropy and enthalpy). Stream 8 is used to preheat stream 6 before the boiler to increase the Ranquine cycle efficiency, while stream 4 is sent to a second turbine of lower operating pressure. The mass ratio between these two stream is a variable of the mathematical model. To determine the energy produced by the second turbine, a similar procedure is performed as for the first turbine, but with the stream 5 at saturation conditions. The operating pressure is set at 0.08 bar (León & Martín, 2016).

Between stream 5 and 6 water condensation is produced using cooling water. The mass of cooling water required can be determined from Eq.(F.17).

$$Hwa_6 - Hw_5 = \frac{F_5}{\lambda} \tag{F.17}$$

F.1.2 *Model of the gasification process*

Following the results of Sanchez et al., 2019, the indirect gasification, which is composed of a gasifier and a combustor is selected to transform grape pomace into energy. In this type of system, the heat required for gasification is supplied by the combustion of the char formed by the gasification process through a heat transfer media (olivine). The mass ratio between the olivine and the dry biomass is 27. In addition, gasification requires 0.4 kg of steam per kilogram of dry biomass (Sanchez et al., 2019). The operating pressure is set at 1.6 bar (Sanchez et al., 2019) while the temperature is a variable of the optimization model. This temperature determines the mole fraction of each component of the syngas (Eqs.(F.18)-(F.24)).

$$y_{CO,syngas} = 133.46 - 0.1029 \cdot T_{syngas} + 0.000028792 \cdot {T_{syngas}}^2 \tag{F.18}$$

$$y_{CO_2,syngas} = -9.5251 + 0.037889 \cdot T_{syngas} - 0.000014927 \cdot {T_{syngas}}^2 \tag{F.19}$$

$$y_{CH_4,syngas} = -13.82 + 0.044179 \cdot T_{syngas} - 0.000046467 \cdot {T_{syngas}}^2 \tag{F.20}$$

$$y_{C_2H_4,syngas} = -38.258 + 0.058435 \cdot T_{syngas} - 0.000019868 \cdot {T_{syngas}}^2 \tag{F.21}$$

$$y_{C_2H_6,syngas} = 11.114 - 0.011667 \cdot T_{syngas} + 0.000003064 \cdot {T_{syngas}}^2 \tag{F.22}$$

$$y_{H_2,syngas} = 17.996 - 0.026448 T_{syngas} + 0.00001893 \cdot T_{syngas}{}^2 \tag{F.23}$$

$$y_{C_2H_2,syngas} = -4.3114 + 0.0054499 \cdot T_{syngas} - 0.000001561 \cdot T_{syngas}{}^2 \tag{F.24}$$

Where $y_{j,syngas}$ is the mole fraction of each component 'j' in the syngas. In addition to the composition of the gas, its amount (mDrySyngas) , as well as the amount of tar (mTar) are also determined from the gasification temperature and equations Eq. (F.25) and Eq.(F.26).

$$mDrySyngas = 28.993 - 0.043325 \cdot T_{syngas} - 0.000020966 \cdot T_{syngas}{}^2 \tag{F.25}$$

$$mTar = 0.045494 - 0.000019759 \cdot T_{syngas} \tag{F.26}$$

The amount of nitrogen, oxygen and sulfur retained by the char is estimated at 6.6%, 8.3% and 4% of that present in the grape pomace, respectively (Sanchez et al., 2019). The carbon retained by the char is determined from the mass balances of the gasification reactor.

An excess of 150% air, together with char, is fed to the combustor at a temperature of 473k. The heat of combustion of the char is estimated at 25000 kJ/kg (Blasi, 2004). In this case, the composition of the flue gas is determined from the material balances at the combustor, assuming complete oxidation of all reactants. For the syngas purification process, a series configuration of two cyclones and an electrostatic precipitator is used. The efficiency of the cyclones is set at 99% for the carbon, ash and olivine and 99.99% (Sanchez et al., 2019) for the electrostatic precipitator. The olivine lost in the cyclones and in the electrostatic precipitator is replaced.

Once the solids have been removed, the syngas goes through 3 stages to make it suitable to produce power. First, a steam reforming stage is used to transform all the hydrocarbons into H_2 and CO. Subsequently, a FeO bed is used to adsorb the H_2S present in the synthesis gas. Finally, a WGSR allows to adjust the H_2/CO ratio to optimize the combustion process in the Bryton cycle (Sanchez et al., 2019).

The reactions considered in the steam reforming process are indicated by Eqs.(F.27)-(F.29).

$$C_nH_m + nH2O \rightarrow nCO + \left(n + \frac{m}{2}\right) H_2 \tag{F.27}$$

$$3H_2 + CO \overset{kp1}{\longleftrightarrow} H_2O + CH_4 \tag{F.28}$$

$$CO + H_2O \overset{kp2}{\longleftrightarrow} H_2 + CO_2 \tag{F.29}$$

All hydrocarbons (C_2H_6,C_2H_4 and C_2H_2), except methane, are completely transformed into CO and H_2. Therefore, both energy and matter balances are modeled from stoichiometric relationships. The conversion of methane is determined from thermodynamic equilibrium, following an empirical relationship (Eq.(F.30)-(F.31)) (Sanchez et al., 2019). These equilibria are controlled by the equilibrium constants kp1 and kp2 which depend on the reaction temperature.

$$kp1 = 10^{\left(-\frac{11650}{T(K)}+13.076\right)} = \frac{P_{CO}\ P_{H_2}^3}{P_{CH_4} P_{H_2O}} \tag{F.30}$$

$$kp2 = 10^{\left(-\frac{1910}{T(K)}-1.784\right)} = \frac{P_{CO_2} P_{H_2}}{P_{CO} P_{H_2O}} \tag{F.31}$$

The maximum temperature is set at 1600K. To determine the amount of iron needed to remove the SH_2 from the synthesis gas, stoichiometric ratios (Eq.(F.32)) and 100% conversion are used (Sanchez et al., 2019).

$$ZnO + H_2S \rightarrow H_2O + ZnS \tag{F.32}$$

A WGSR is used to adjust the H2/CO ratio to an optimal value to maximize energy production. Eq.(F.30)-(F.31) are used for the composition of the flue gas. The gas is compressed to 4.5 bar, which causes an increase in gas temperature, according to the Eq.(F.33)

$$T_{out} = T_{in} + T_{in} \cdot (P_{out}/P_{in})^{((z-1)/z)-1} \cdot \frac{1}{nc} \tag{F.33}$$

Therefore, it is necessary to cool it down to 25ºC to feed the PSA tower. This causes the condensation of most of the water contained in this stream. The amount condensed is determined from Rault, Dalton and Antony's law. A PSA system is used to retain the remaining moisture, CO and up to 95% of the CO_2 (León & Martín, 2016). Once the synthesis gas is purified, it is used to produce electrical energy from a Brayton cycle, whose modeling is shown in Section F.1.3.

F.1.3 *Model of the anaerobic digestion process*

The feed stream is mixed with a water stream until a solids concentration of 10% is reached. Most of the water used in this stage is recovered at the end of the process, in the dehydration of the digestate. This not only saves water, but it also helps the anaerobic digestion process by acting as an inoculum for the biological reaction. The output stream is heated to 37ºC ($T_{digestion}$) to achieve the optimal digestion conditions (Taifouris & Martín, 2018). The mass and energy balances are shown by Eqs.(F.34)-(F.36).

$$f_{H_2O,feed} = (f_{Lipids,feed} + f_{Ch,feed} + f_{Prot,feed} + f_{Ash,feed} + f_{NH_3,feed} + f_{Rest,feed}) \cdot 0.10 \tag{F.34}$$

$$Q_{preheating} = F_{steam1} \cdot \lambda_{steam} \tag{F.35}$$

$$Q_{preheating} = F_{feed} \cdot Cp_{H2O} \cdot (T_{digestion} - Tref) \tag{F.36}$$

Where $f_{lipids,feed}$,$f_{ch,feed}$,$f_{Prot,feed}$,$f_{Ash,feed}$, and $f_{NH_3,feed}$ are the mass flows of lipids, carbohydrates, protein, ash and inorganic nitrogen in the feed, while $f_{rest,feed}$ is the non-reaction biomass of the waste, λ_{steam} is the heat of vaporization of the steam and Cp_{H2_2O} is the heat capacity of the water. It is considered that the heat capacity of the mixer output stream will be similar to the heat capacity of the water since 90% of this stream is water. Both variables depend on the temperature, as can be seen in the literature (Sinnot, 2005a). T_{ref} is the reference temperature (25ºC) and F_{feed} is the total feed mass.

For the modeling of anaerobic digestion process of the grape pomace, the model present in the work of Taifouris and Martín, 2023a is used. For this purpose, the stoichiometric ratios of fats, proteins and carbohydrates are used, following Eqs.(F.37)-(F.40) and Eqs.(F.44-F.46).

$$f_{CH_4,digestor} = 0.6588 \cdot fLir + 0.2433 \cdot fCHr + 0.2383 \cdot fPrr \tag{F.37}$$

$$f_{CO_2,digestor} = 0.6644 \cdot fLir + 0.6675 \cdot fCHr + 0.6822 \cdot fPrr \tag{F.38}$$

$$f_{NH_3,digestor} = 0.0280 \cdot fLir + 0.0227 \cdot fCHr + 0.1647 \cdot fPrr \tag{F.39}$$

$$f_{H_2O,digestor} = -0.4810 \cdot fLir - 0.039 \cdot fCHr - 0.2047 \cdot f\Pr r \tag{F.40}$$

Eq.(F.41) determines the amount of cell mass that is generated in the process.

$$f_{bat,digestor} = 0.1857 \cdot fLir + 0.1508 \cdot fCHr + 0.1241 \cdot f\Pr r \tag{F.41}$$

Therefore, the mass of the biogas and the digestate is calculated by Eqs.(F.42)-(F.43)

$$F_{biogas} = f_{CH4,digestor} + f_{CO2,digestor} + f_{NH3,biogas} + f_{H2O,biogas} \tag{F.42}$$

$$\begin{aligned} F_{digestate} = &\left(f_{lipids,feed} + f_{ch,feed} + f_{prot,feed}\right) \cdot 0.5 \\ &+ f_{rest,feed} + f_{NH3,digestate} + f_{H2O,digestate} \end{aligned} \tag{F.43}$$

From experimental data obtained from grape pomace biodegradability, an average biodegradability of 0.5 (Converti et al., 1999; Rao & Singh, 2004; Liu et al., 2009; Bah et al., 2014; Zhang et al., 2014; Nielfa et al., 2015) is considered for all compounds (Eqs.(F.44)-(F.46)).

$$fCHr = f_{ch,feed} \cdot 0.5 \tag{F.44}$$

$$fLir = f_{Li,feed} \cdot 0.5 \tag{F.45}$$

$$f\Pr r = f_{Prot,feed} \cdot 0.5 \tag{F.46}$$

The thermodynamic equilibrium is used to estimate the distribution of H_2O and NH_3, between the gas and liquid phases (the rest of the gases can be considerded insoluble according to Henry's constants (Sinnot, 2005a)), by using the laws of Dalton, Raoult and Antoine (Eqs.(F.47)-(F.51)).

$$y_{NH_3,biogas} = Pv_{NH_3} \cdot x_{NH_3,digestate} \tag{F.47}$$

$$y_{H_2O,biogas} = \frac{MW_{H_2O}}{MW_{biogas-dry}} \cdot \frac{Pv_{H_2O}}{Pt_{Digestion} - Pv_{H_2O}} \tag{F.48}$$

$$MW_{biogas-dry} = \sum_i y_{i,biogas} \cdot MW_i \quad \forall i \in \{i = CH_4, CO_2, NH_3\} \tag{F.49}$$

$$\sum_i x_{i,digestate} = 1 \quad \forall i \in \{i = bat, lip, ch, prot, lig, ash, NH_3, H_2O, rest\} \tag{F.50}$$

$$\sum_i y_{i,biogas} = 1 \quad \forall i \in \{i = CH_4, CO_2, NH_3, H_2O\} \tag{F.51}$$

Where $y_{j,biogas}$ is the mole fraction of component 'j' in the biogas (gas phase) and $x_{j,biogas}$ is the mole fraction of component 'j' in the digestate (liquid phase). MW_i is the molecular mass of component 'i' (CH_4,CO_2,NH_3,Biogas or Water). Pv_{H_2O} is the vapor pressure of the water and Pt is the operating pressure of the digestion, which is , one bar. Once the mole fractions of water and ammonia in the liquid and gas phase are calculated, and the total mass of each of the phases is known, the amount of each of these chemical compounds in both phases can be determined (Eqs.(F.52)-(F.57)).

$$f_{NH3,biogas} = y_{NH_3,biogas} \cdot N_{biogas} \cdot MW_{NH_3} \tag{F.52}$$

$$f_{NH3,digestate} = x_{NH_3,digestated} \cdot N_{digestate} \cdot MW_{NH_3} \tag{F.53}$$

$$f_{H_2O,biogas} = y_{H_2O,biogas} \cdot N_{biogas} \cdot MW_{H_2O} \tag{F.54}$$

$$f_{H_2O,digestate} = x_{H_2O,digestate} \cdot N_{digestate} \cdot MW_{H_2O} \tag{F.55}$$

$$N_{biogas} = \sum_i \frac{f_{i,biogas}}{MW_i} \quad \forall i \in \{i = CH_4, CO_2, NH_3, H_2O\} \tag{F.56}$$

$$N_{digestate} = \sum_i \frac{f_{i,digestate}}{MW_i} \quad \forall i \in \{i = bat, lip, ch, prot, lig, ash, NH3, H2O, rest\} \tag{F.57}$$

Where N_{biogas} is the total moles of the gas stream (biogas), and $N_{digestate}$ are the total moles of the liquid stream (digestate). The volume of biogas (V_{biogas}), assuming ideal gas, is estimated by Eq.(F.58)

$$V_{biogas} = \frac{0.082\frac{atm \cdot l}{mol \cdot k} \cdot 310K \cdot (\sum_i \frac{m_{i,biogas}}{MW_i})}{Pt_{Digestion}} \forall i \in \{i = CH_4, CO_2, NH_3, H_2O\} \tag{F.58}$$

The composition of the digestated is estimated through a mass balance between the compounds that enter the digester with the raw material (see Table F.3) and those that leave this equipment with the biogas (Eqs(F.59)-(F.65)).

Table F.3: Composition of the Grape pomace (RM: raw material)

	g/KgRM	**References**
TS	434	(Achkar et al., 2016)}
VS	394	
Total Nitrogen	7	
Phosphorous	2	
Water	566	
Lipids	62	(Almeida et al., 2021)
Carbohydrates	220	
Protein	107	
N-NH4+	0.4	(Javier et al., 2019)
Potasium	13	(Juráček et al., 2021)
Polyphenols	32	(Jin et al., 2021a)
Tannis	96	Llobera and Cañellas, 2007

$$f_{C,digestate} = f_{C,feed} - f_{CH_4,biogas} \cdot \frac{MW_C}{MW_{CH_4}} - f_{CO_2,biogas} \cdot \frac{MW_C}{MW_{CO_2}} \tag{F.59}$$

$$f_{N_{org}, digestate} = f_{Norg,feed} \tag{F.60}$$

$$f_{N_{am}, digestate} = f_{Nam,feed} - f_{NH3, biogas} \cdot \frac{MW_N}{MW_{NH3}} \tag{F.61}$$

$$f_{P,digestate} = f_{P,feed} \tag{F.62}$$

$$f_{K,digestate} = f_{K,feed} \tag{F.63}$$

$$f_{REST, digestate} = f_{REST, feed} \tag{F.64}$$

$$f_{H2O,digestate} = f_{H2O,feed} - F_{biogas} \cdot y_{H_2O,biogas} \tag{F.65}$$

The heat required to maintain the anaerobic digestion reaction and keep the reactants in mesophilic conditions is determined from an empirical factor (Wu et al., 2015) which relates the heat required to the volatiles solids reacting (3.6 kJ per gram of volatile solid degraded).

The biogas must be upgraded before being fed to the Brayton cycle. First, the H_2S must be removed. For this, an iron oxide bed is used, which reacts with H_2S producing produces iron sulfide and water, assuming 100% conversion (Sanchez et al., 2019). A PSA system with a 5A zeolite packed bed is used to completely remove CO, NH_3, and H_2O. 95% of the CO_2 is also retained (León & Martín, 2016). This process is carried out at a pressure of 4.5 bar and 25ºC. The digestate is dehydrated by using a filter, dried up to 10% moisture and stored (Taifouris & Martín, 2018).

A Brayton cycle is proposed to produce energy from the combustion of the biomethane produced. The use of a combined cycle is discarded since the combustion gases are to be used to supply the energy needed for the digestion process. The combustion process is modeled from stoichiometric ratios based on methane combustion, considering a 100% conversion. A 150% excess of air with respect to the stoichiometric ratio is used (Eq.(F.66)). The atomic balances, explained at the beginning of section F.1.1, can be used to estimate the balance of matter in this combustion process.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2\,O \tag{F.66}$$

Since this is a combustion process, the energy balances shown in Section F.1.1 can be used to estimate the flue gas outlet temperature, but taking into account that in this case methane is combusted.

On the one hand, the electrical energy needed to compress the biogas before the combustion process and that produced in the turbine, due to the expansion of the combustion gases, is determined from Eq.(F.67).

$$W = F + \frac{R \cdot z \cdot T_{in}}{MW \cdot (k-1)} \cdot \left(\frac{P_{out}}{P_{in}}\right)^{\frac{(k-1)}{k}-1} \cdot \frac{1}{nc} \tag{F.67}$$

Where k is the polytropic coefficient (1.4), nc is the compressor or turbine efficiency (0.85). T_{in} is the inlet temperature, P_{out} is the inlet pressure, and P_{in} is the inlet pressure.

On the other hand, the temperature of the gases at the outlet of the compressors and the turbines is calculated from Eq.(F.68)

$$T_{out} = T_{in} + T_{in} \cdot (P_{out}/P_{in})^{((z-1)/z)-1} \cdot \frac{1}{nc} \tag{F.68}$$

The turbine exhaust gases are used to supply heat to the bioreactor.

F.1.4 *Model of the pyrolisis*

Due to the large number of chemical and physical reactions that occur in the pyrolysis process of a waste, we proceeded to model them using empirical yields from the literature. According to the work of Ateş et al., 2019 for the pyrolysis of 1 kg of dried grape pomace, 0.31 kg of biochar, 0.31 kg of bio-oil and 0.38 kg of gas are generated. The composition of each of the phases is also estimated from empirical data (Ateş et al., 2019).

To perform the pyrolysis process it is necessary to heat the raw material to the optimum reaction conditions, that is, 500°C and to supply the heat necessary to carry out the chemical and physical reactions and maintain the isothermal system, since the process is endothermic. For this purpose, the flue gases from the bio-oil combustion process and the gas produced in the pyrolysis are used. In this way, the process is auto-thermal. The energy balance that determines the flue gas outlet temperature is shown by Eq. (F.69)

$$\sum_j (CpFG_j \cdot NFG_j) = \sum_j (CpRM_j \cdot NRM_j) + Qpyro \tag{F.69}$$

Where $CpFG_j$ the integration of the specific heat variations between the inlet and outlet temperatures of the flue gas (Eq. (F.69)), $CpRM_j$ is the integration of the specific heat variations between the inlet and outlet temperatures of the raw material (Eq. (F.69)), while NFG_j and NRM_j are the moles of the flue gas and raw material, respectively. The heat required to keep the reaction isothermal (Qpyro) is estimated from the work of Xu et al., 2009 and its value is 1930 J/g biomass feed.

$$CpFG_j = A_j(TFGout - TFGin) + B_j \cdot \frac{1}{2} \cdot (TFGout - TFGin)^2 + \\ C_j \cdot \frac{1}{3} \cdot (TFGoutTFGin)^3 + D_j \cdot \frac{1}{4} \cdot (TFGout - TFGin)^4 \tag{F.70}$$

$$CpRM_j = A_j(TRMout - TRMin) + B_j \cdot \frac{1}{2} \cdot (TRMout - TRMin)^2 + \\ C_j \cdot \frac{1}{3} \cdot (TRMout - TRMin)^3 + D_j \cdot \frac{1}{4} \cdot (TRMout - TRMin)^4 \tag{F.71}$$

Where A_j,B_j, C_j and D_j are empirical factors to estimate the specific heat of the raw material and depend on the compound 'j' of the grape pomace.

The gas and bio-oil are used to produce energy to dry the raw material entering the process. For this, it is necessary to determine the amount of energy that can be obtained from these products, via combustion. The composition of the gas as well as the elemental composition of the bio-oil are shown in the following tables (F.4) y (F.5) respectively.

Table F.4: Composition of the gas generated by the pyrolisis of the grape pomace (Ateş et al., 2019)

Component	**wt%**
H2	8.00
CH4	8.00
CO	28.00
CO2	56.00

Table F.5: Ultimate analysis of bio-oils generated by the pyrolisis of the grape pomace (Ateş et al., 2019).

Component	**wt%**
C	69.28
H	7.82
N	2.33
O	20.57

On the one hand, from the elemental composition, it is possible to obtain the empirical formula of bio-oil, which is as follows $CH_{1.33}O_{0.179}N_{0.032}$. Using the procedure described in Section F.1.1, it is possible to determine the amount of energy that can be released in the bio-oil combustion process (in this case all the heat goes to heat the flue gas). On the other hand, from the composition of the gas, the energy released in the combustion process can be determined, following the procedure described in Section F.1.3 for the synthesis gas, but taking into account that this gas, in addition to methane, also contains H_2 and CO. Therefore, two more oxidation reactions should be added. (Eqs.(F.72)-(F.73)).

$$H_2 + 1/2O_2 \rightarrow 2H_2\,O \tag{F.72}$$

$$CO + 1/2O_2 \rightarrow CO_2 \tag{F.73}$$

These gases are combined and the equilibrium temperature is determined from energy balances (Eq.F.74).

$$\sum_j (Cpout_j \cdot Nout_j) = \sum_j (Cpin1_j \cdot Nin1_j + Cpin1_j \cdot Nin2_j) \tag{F.74}$$

Where $Nin1_j$ and $Nin2_j$ are the moles of each compound 'j' of each input stream (gases from the combustion of bio-oil and gases from the combustion of the gas generated in pyrolysis), while that $Nout_j$ are the moles of each compund 'j' of of the mixer outlet gas. $Cpin1_j$, $Cpin2_j$ and $Cpout_j$ are the specific heats of the input and output streams and are calculated from Eqs.(F.75-F.77)

$$\begin{aligned} Cpout_j &= A_j(Tout - Tref) + B_j \cdot \frac{1}{2} \cdot (Tout - Tref)^2 + \\ C_j \cdot \frac{1}{3} &\cdot (Tout - Tref)^3 + D_j \cdot \frac{1}{4} \cdot (Tout - Tref)^4 \end{aligned} \tag{F.75}$$

$$\begin{aligned} Cpin1_j &= A_j(Tin1 - Tref) + B_j \cdot \frac{1}{2} \cdot (Tin1 - Tref)^2 \\ &+ C_j \cdot \frac{1}{3} \cdot (Tin1 - Tref)^3 + D_j \cdot \frac{1}{4} \cdot (Tin1 - Tref)^4 \end{aligned} \tag{F.76}$$

$$\begin{aligned} Cpin2_j &= A_j(Tin2 - Tref) + B_j \cdot \frac{1}{2} \cdot (Tin2 - Tref)^2 + C_j \cdot \\ \frac{1}{3} &\cdot (Tin2 - Tref)^3 + D_j \cdot \frac{1}{4} \cdot (Tin2 - Tref)^4 \end{aligned} \tag{F.77}$$

The resulting gas is used to dry the feedstock since pyrosilis requires the feedstock to be dried (10% moisture) and grape pomace contains slightly more than 50% moisture (Rodrigues et al., 2022).

F.1.5 *Integrated multyproduct system*

The integrated multi-product system is composed of 3 different process lines, the production of oil, polyphenols and biochar. It is an integrated system in which the residues from one process are used to produce a new product in the next line. Thus, polyphenols are produced from the residues of the oil production line, while biochar is produced from the residues of the polyphenol production process. The process is modeled by means of material and energy balances that can be derived from the work of Jin et al., 2021a.

F.1.5.1 *Production of oil*

First, the feedstock is dried using flue gas generated from the combustion of part of the grape pomace. This stage is modeled following the procedure described in Section F.1.6. Subsequently, the seeds are separated from the skins. The separation ratio between seeds and skins is 16:9. The seeds are sent to the extration process to obtain their oil. The first step is to heat the inlet stream up to the extraction temperature, that is 60 °C. For this purpose, a steam, which is generated together with the flue gas in the combustion of the grape pomace, is used.

The energy balance is indicated by Eq.(F.78).

$$\begin{aligned} m_{steam} \cdot \lambda_{H_2O} &= Fseed \cdot x_{seed} \cdot (A_j \cdot (Tseedout - Tseedin) \\ &+ 1/2 \cdot B_j \cdot (Tseedout^2 - Tseedin^2) + \\ &1/3 \cdot C_j \cdot (Tseedout^3 - Tseedin^3) + 1/4 \cdot D_j \cdot (TFout^4 - Tseedin^4)) \end{aligned} \tag{F.78}$$

Where Fseed is the flow rate of the stream containing the seeds, while x_{seed} is the composition of the seeds in terms of lipids, carbohydrates, protein, fiber and ash. The terms A_j,B_j,C_j and D_j are the same as those used for drying grape pomace in the Section F.1.6. Tseedout is 60°C while $T_{seeedin}$ is 25°C.m_{steam} is the mass of vapor and λ_{H2O} is the latent heat of water.

The oil extraction process is carried out by hexane, at a ratio of 3:1 with respect to the stream containing the seed. From the equipment design data presented in the supplementary material to the work of Jin et al., 2021a, the ratio of the input to output streams can be deduced. By analyzing the total concentration of oil in the seed, the stream ratio and the extraction yield (0.987), it is determined that up to 0.146 kg of oil can be obtained per kg fed to the extractor. From the annual hexane consumption presented in the results of the Jin et al., 2021a work, it can be determined that the amount of hexane to be introduced into the process is 0.0057kg per kg of raw material. Most of the hexane is recovered in the solvent recovery process. 0.6714 kg of water is lost per kg of hexane. From the oil extracted and the amount of hexane lost, the amount of residue generated at this stage is computed using a global mass balance in the extractor. This residue is mixed with the skins and sent to the polyphenol production line.

The oil stream is heated up to 80ºC following a procedure similar to the one indicated in Eq.(F.78). But in this case, only parameters A,B,C,D corresponding to lipids are considered. Subsequently, the oil is washed with water (0.3kg of H_2O per kg of oil) and NaOH (0.2kg per kg of oil). 16.83% of the scrubber output stream is separated as solid residue. The remaining residue is separated after the second wash. This second wash is performed with water (0.1 kg of H_2O per kg of oil) at 60ºC. The stream containing the oil is dried following the procedure described in Section F.1.6 and fed to the bleaching tank, where 0.03 kg of clay is fed per kg of oil. A filter is used to remove the spent clay (1.036 kg of spend clay is removed per kg of clay added to the system). Finally, the oil is subjected to a deodorization process by increasing its temperature up to 230ºC. This process is carried out by a fire heater fed with part of the raw material. To determine the amount of grape pomace to be combusted, Eq. (F.79) is used.

$$\begin{aligned} f_{GP} \cdot Qcomb = F_{oil} \cdot (A_{oil} \cdot (230 - 115) + 1/2 \cdot B_{oil} \cdot (230^2 - 115^2) \\ +1/3 \cdot C_{oil} \cdot (230^3 - 115^3) + 1/4 \cdot D_{oil} \cdot (230^4 - 115^4)) \end{aligned} \tag{F.79}$$

Where Qcomb is the heat of combustion which can be determined using the procedure described in Section F.1.1 while f_{GP} is the mass of grape pomace used as fuel.

F.1.5.2 *Production of polyphenols*

The residues proceeding from the oil extraction line are heated up to the optimum extraction conditions, that is, up to 70ºC. The energy balances are similar to those shown by Eq.(F.78). In this case, the extraction is carried out through a 40% ethanol solution. The ethanol must also be heated to 70ºC. The ethanol feed ratio is 5:1 with respect to the waste feed. Through the equipment design of the supplementary material of the work of Jin et al., 2021a , it is possible to determine the amount of material that goes to the evaporator and the amount that goes to the mixer. The 63.67% of the extractor output stream continues the polyphenol production line, as it is the polyphenol-rich stream, while the residual stream is sent to a mixer, where it will join the residue from the next extraction.

The polyphenol-rich stream is sent to an evaporator to recover part of the ethanol used. After the evaporation process, 94.1% of the total stream is evaporated (this stream is considered to contain only ethanol and water). It is also known that the non-evaporated part has been enriched by 65% in solid components, so that the remaining 35% is water.

The global balance at the evaporator, which is necessary to determine the mass of steam needed for the vaporization process, is shown by Eq.(F.80).

$$\begin{aligned}(Qoutgas + Qoutliq + Qpoly) - (Qinliq) = \\ m_{steameva1} \cdot 525.7kcal/kg \cdot 4.18kj/kcal\end{aligned} \tag{F.80}$$

Where Qoutgas, Qoutliq and Qinliq are the enthalpy of the outlet gaseous stream, outlet liquid stream and inlet liquid stream, respectively. The enthalpy calculation of each of these streams is shown by Eq.(F.81)-(F.83). The evaporator outlet temperature (97°C) can be estimated from the composition of the gaseous and liquid streams, assuming an ethanol-water system reaching thermodynamic vapor-liquid equilibrium.

$$\begin{aligned}Qoutgas = \sum_j Foutgas_j \cdot (A_j \cdot (Tout - Tref) + 1/2 \cdot B_j \cdot (Tout^2 - Tref^2) + \\ 1/3 \cdot C_j \cdot (Tout^3 - Tref^3) + 1/4 \cdot D_j \cdot (Tout^4 - Tref^4))\end{aligned} \tag{F.81}$$

$$\begin{aligned}Qoutliq = \sum_j Foutliq_j \cdot (A'_j \cdot (Tout - Tref) + 1/2 \cdot B'_j \cdot (TEout^2 - Tref^2) + \\ 1/3 \cdot C'_j \cdot (TEout^3 - Tref^3) + 1/4 \cdot D'_j \cdot (TFout^4 - Tref^4))\end{aligned} \tag{F.82}$$

$$\begin{aligned}Qinliq = \sum_j Fin_j \cdot (A'_j \cdot (Tin - Tref) \cdot +1/2 \cdot B'_j \cdot (Tin^2 - Tref^2) + \\ 1/3 \cdot C'_j \cdot (Tin^3 - Tref^3) + 1/4 \cdot D'_j \cdot (Tin^4 - Tref^4))\end{aligned} \tag{F.83}$$

Parameters A,B,C,D are the empirical parameters related to the specific heat of gases while A′,B′,C′, and D′ are the parameters related to the specific heat of liquids. These empirical parameters can be found in the literature (Sinnot, 2005a). Qpoly is the heat absorbed by the polyphenols, which is determined by the correlation shown by Eq.(F.84) (Erkac & Yigitarslan, 2021).

$$Qpoly = (0.1243 \cdot Tout + 303.69) \cdot Finpoly/138.12 \cdot (Tout - Tin) \quad \text{(F.84)}$$

In this second extraction step, a 95% ethanol stream is used to purify the polyphenol stream. In this case, 0.5 kg of ethanol is added per kg of feed. From the extractor output, 56.8% continues with the polyphenol production line while the rest is considered waste and sent to a mixer, where it is mixed with the residual output of the first extractor. This purification process allows 65% of the impurities to be precipitated (Jin et al., 2021a). As the total amount of polyphenols is known (0.0319 kg per kg of dried grape pomace) and also its extraction yield (82.8%), the amount of impurities in the stream can be determined. Since this piece of equipment is a splitter, water and ethanol are considered to be distributed in the same proportion in the solid phase as in the liquid phase, in order to reduce the degrees of freedom in determining the composition of the streams.

The polyphenol-rich stream is fed to an evaporator to recover the ethanol used. The 58.59% of the fed stream is sent to a dryer (polyphenol-rich stream) and the rest (ethanol and water) are mixed with the gaseous output of the previous evaporator. Mass balances to this evaporator are modeled like the previous evaporator. The polyphenols must be dried to 7% moisture. The drying process is modeled as indicated in Section F.1.6. The polyphenol-rich dryer output stream constitutes 73.72% of the dryer feed stream, while the remainder is the matter removed by the flue gas.

The residues from the extractions are sent to a desolventizer to recover ethanol. The yield of the desolventizing process is 80%. After this step, 34% of the input stream is evaporated, while the rest, composed of solid residue, is sent to a drying process. All gaseous streams of water and ethanol are blended and sent to the ethanol recovery line. These streams are cooled using cooling water and then distilled to obtain a 95% ethanol stream. A portion of this stream is used for the purification stage of the polyphenol extraction process, while the remainder is diluted with water to 40% to extract the polyphenols.

F.1.5.3 *Production of biochar*

After the desolventizing process, the residues are cooled from 89°C to 60°C, dried to a humidity of 2% and fed to the pyrolysis reactor. The pyrolysis process is modeled as indicated in Section F.1.4 .

F.1.6 *Drying of the raw material*

For the combustion, gasification, pyrolysis and IMPS processes it is necessary to dry the feedstock.

For this, either the products of the process are used to generate heat (auto-thermal process) or part of the grape pomace is combusted to utilize the heat generated. A priori it is not known exactly which processes are autothermal and which are not, and therefore, in all drying processes the possibility of using a certain amount of raw material as fuel is considered.

The raw material outlet conditions are set at 50ºC and 10% humidity for all processes. Therefore, the temperature of the flue gas can not be lower than 60ºC and its maximum relative humidity cannot exceed 90%.

The mass balances are shown by the Eq.(F.85)-(F.87).

$$F_{FG_{in}} = F_{FG_{out}} \quad j \neq H_2O \tag{F.85}$$

$$F_{RMin} = F_{RMout} \quad j \neq H_2O \tag{F.86}$$

$$F_{FG_{out}} = F_{FGin_j} + (F_{RMout_j} - F_{RMin_j}) \;\; j = H_2O \tag{F.87}$$

The general energy balance in the drying process is shown by Eq.(F.88).

$$QinFG + QinRM = QoutRM + QoutFG \tag{F.88}$$

The raw material comes into contact with the flue gas, increasing its temperature up to a maximum of 50ºC. It is considered that only water is removed from the grape pomace. The energy balances at the inlet and outlet of the dryer applied to the grape pomace (QinFG and QoutFG, respectively) are shown by Eqs.(F.89)-(F.90).

$$\begin{aligned} QinRM = xin_j \cdot FRMin \cdot (A_j \cdot (TRMin - TRMref) + \\ B_j \cdot 1/2 \cdot ((TRMin - 273)^2 - (TRMref - 273)^2) - \\ C_j \cdot 1/3 \cdot ((TRMin - 273)^3 - (Tref - 273)^3)) \;\; j = H2O \end{aligned} \tag{F.89}$$

$$QoutRM = xout_j \cdot FRMout \cdot (A_j \cdot (TRMout - Tref) \\ + B_j \cdot 1/2 \cdot ((TRMout - 273)^2 - (Tref - 273)^2) - \\ C_j \cdot 1/3 \cdot ((TRMout - 273)^3 - (Tref - 273)^3)) \quad j = H2O \tag{F.90}$$

The parameters A_j,B_j,and C_j are empirical parameters that can be consulted in the literature (Becker & Fricke, 2003) and depend on the type of grape pomace component (protein, carbohydrate, lipids, etc). TRMin and TRMout are the inlet and outlet temperature of the grape pomace, respectively. FRMin and FRMout are the grape pomace inlet and outlet mass flow rates. Finally, xin_j and $xout_j$ are the composition of grape pomace (lipids, carbohydrates, protein, etc.) at the inlet and outlet.

The mass balances of the flue gas, inlet and outlet of the dryer are shown by the Eq.(F.91)-(F.92).

$$QFGin = A'_j \cdot (TFGin - Tref)) + ((1/2) \cdot B'_j \cdot (TFGin^2 - Tref^2)) + \\ ((1/3) \cdot C'_j \cdot (TFGin^3 - Tref^3)) + ((1/4) \cdot D'_j \cdot (TFGin^4 - Tref^4)) \cdot NFGinj \tag{F.91}$$

$$QFGout = A'_j \cdot (TFGout - Tref) + ((1/2) \cdot B'_j \cdot (TFGout^2 - Tref^2)) \\ + ((1/3) \cdot C'_j \cdot (TFGout^3 - Tref^3)) + ((1/4) \cdot D'_j \cdot (TFGout^4 - Tref^4)))) \\ \cdot (xout_{H2O} \cdot FRMout - xin_{H2O} \cdot FRMin) \cdot \lambda_{H_2O} \tag{F.92}$$

The parameters A'_j,B'_j,and C'_j, D'_j are empirical parameters associated with each component of the flue gas (CO_2,N_2,O_2, or H_2O) and can be found in the literature (Sinnot, 2005a). TFG_{in} and TFG_{Out} are the flue gas inlet and outlet temperature, respectively. $NFGin_j$ and $NFGout_j$ are the moles of each flue gas component at the inlet and outlet of the dryer.

For the gas used to dry the grape pomace, two requirements must be met, its temperature must not fall below 60°C and its relative humidity (ϕ) must not exceed 90%. To determine the relative humidity, the Eqs.(F.93)-(F.95) are used. This is obtained by combining Raoult's, Antoine's and Dalton's law, as well as the ideal gas equation.

$$Pa = \frac{MWgas}{18 \cdot \sum_j F_{FG_j} - F_{FG_{H_2O}}} \cdot (Pt - Pa) \cdot (F_{FG_{H_2O}}) \tag{F.93}$$

$$Ps = 10^{A - \frac{B}{T(C)+C}} \tag{F.94}$$

$$\phi = \frac{Pa}{Ps} \tag{F.95}$$

Those processes that do not meet these two requirements must use another heat source to dry the raw material. To consider these cases, the Eq.(F.88) is modified to Eq.(F.96).

$$QinFG + QinRM = QoutRM + QoutFG + Qextra \tag{F.96}$$

Where Qextra is the heat required to achieve the drying conditions. This heat is minimized by adjusting the flue gas exit conditions to the more restrictive of the two conditions presented above.

$$\begin{aligned} Qextra = \; & Fextra \cdot (A'j \cdot (TEout - TEin) + 1/2 \cdot B' \cdot (TEout^2 - TEin^2) + \\ & 1/3 \cdot C' \cdot (TEout^3 - TFGin^3) + 1/4 \cdot D' \cdot (TFout^4 - TFGin^4)) \end{aligned} \tag{F.97}$$

Fextra is the amount of flue gas required to complete the drying process, which is generated with a part of the feedstock, from the combustion process described in Section F.1.1. TEout and TEin are the outlet and inlet temperatures of this flue gas.

F.1.7 *CAPEX estimation of the processes considered*

It it necessary to calculate the CAPEX of the factory to estimate the fixed operating cost (Sinnot, 2005b). CAPEX is estimated following different procedures depending on each process:

- Combustion and tannin production process: The cost of each piece of equipment is estimated using the empirical correlations shown in the work of Couper et al., 2005.
- Gasification: The reactors for the water gas shift reaction, ZnO absorption, steam reforming and gasification process are estimated following the methodology shown in the work of Sánchez et al., 2019. The cost estimation of filters, cyclones and electric precipitator is developed following the work of Almena and Martín, 2016. The rest of the equipment, such as heat exchangers, compressor or furnaces, are estimated following the work of Couper et al., 2005.

- Anaerobic Digestion: The cost of the digester is calculated following the cost estimation described in the work of Taifouris and Martín, 2023b. All other equipment is estimated following the work of Couper et al., 2005.

- Pyrolisis: The cost is estimated from the plant capacity and the empirical correlation (Eq.(F.98)) from the work of Ramos and Ferreira, 2022.

$$CAPEX_{pyrolisis}(€) = 1973.25 \cdot F\left(\frac{drykg}{h}\right) \cdot \left(\frac{CEPCI_{2023}}{CEPCI_{2022}}\right) \tag{F.98}$$

- IMPS: Both for the single oil production and for the process that also integrates the production of polyphenols and biochar, the procedure used is described in the work of Jin et al., 2021b and consists of a capacity ratio (Eq.(F.99)) for the oil production and (Eq.(F.100)) for the polyphenols production .

$$CAPEX_{oil}(MMe) = 14.6 \cdot \left(\frac{F(t/year)}{32659}\right)^{0.6} \cdot \left(\frac{CEPCI_{2023}}{CEPCI_{2021}}\right) \tag{F.99}$$

$$CAPEX_{polyphenols}(MMe) = 37.7 \cdot \left(\frac{F(t/year)}{32659}\right)^{0.6} \cdot \left(\frac{CEPCI_{2023}}{CEPCI_{2021}}\right) \tag{F.100}$$

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G

APPENDIX G: SUPPLEMENTARY INFORMATION OF CHAPTER 9

G.1 FRAMEWORK DEVELOPMENT

The following sections present models to minimize the biomethane production cost obtained through the anaerobic digestion and gasification processes.

G.1.1 *Modeling of Anaerobic digestion process*

This model is a combination of the work of Taifouris and Martín, 2018 and Erick León, 2016, and is used to estimate the amount and composition of the biomethane obtained from waste. Additionally, it allows estimating the distribution of H_2O and NH_3 between the liquid and gas phases in the digestor, as well as the composition of digestate. The last part of the model is focused on modeling biogas upgrading.

First, the amount of water to reach the conditions of the anaerobic digestion process (Taifouris & Martín, 2018), that is, a solids concentration of 10% is calculated by Eq.(G.1).

$$m_{H_2O,feed} = (m_{lipids,feed} + m_{ch,feed} + \\ m_{prot,feed} + m_{ash,feed} + m_{NH_3,feed} + m_{rest,feed}) \cdot 0.10 \tag{G.1}$$

Where $m_{rest,feed}$ is the non-reaction biomass of the waste.

In addition, it is necessary that the mixture of waste and water enter the reactor under mesophilic conditions, with a temperature of 37°C (Taifouris & Martín, 2018). To do this, steam is used. The amount of steam is calculated by Eqs.(G.2)-(G.3) .

$$Q_{preheating} = m_{steam1} \cdot \lambda_{steam} \tag{G.2}$$

$$Q_{preheating} = M_{feed} \cdot Cp_{H2O} \cdot (T_{digestion} - Tref) \tag{G.3}$$

Where λ_{steam} is the latent heat of water and Cp_{H_2O} is the heat capacity of the water. Since the most of mixture is water, the heat capacity of water is used. Both variables depend on the temperature, as can be seen in the literature (Perry & Green, 1997).

Only a part of the lipids, carbohydrates, and proteins react, depending on their biodegradability. Analyzing the average biodegradability of these components according to the literature (Converti et al., 1999; Rao & Singh, 2004; Liu et al., 2009; Bah et al., 2014; Zhang et al., 2014; Nielfa et al., 2015), it is considered that approximately 50% of the lipids, carbohydrates, and proteins are degraded (Eqs.(G.4), (G.5), and (G.6)).

$$mCHr = m_{ch,feed} \cdot 0.5 \tag{G.4}$$

$$mLir = m_{Li,feed} \cdot 0.5 \tag{G.5}$$

$$m\,\mathrm{Pr}\,r = m_{Prot,feed} \cdot 0.5 \tag{G.6}$$

Once the biodegradability is established, the amount of products generated is determined from stoichiometric ratios (Taifouris & Martín, 2018), so that the Eqs (G.7)-(G.10) determine the amount of CH_4, CO_2, NH_3 , H_2O and biomass formed in the reaction.

$$m_{CH_4,digestor} = 0.6588 \cdot mLir + 0.2433 \cdot mCHr + 0.2383 \cdot mPrr \tag{G.7}$$

$$m_{CO_2,digestor} = 0.6644 \cdot mLir + 0.6675 \cdot mCHr + 0.6822 \cdot mPrr \tag{G.8}$$

$$m_{NH_3,digestor} = 0.0280 \cdot mLir + 0.0227 \cdot mCHr + 0.1647 \cdot mPrr \tag{G.9}$$

$$m_{H_2O,digestor} = -0.4810 \cdot mLir - 0.039 \cdot mCHr - 0.2047 \cdot m\,\mathrm{Pr}\,r \tag{G.10}$$

Eq.(G.11) determines the amount of biomass that is generated in the reaction.

$$m_{bat,digestor} = 0.1857 \cdot mLir + 0.1508 \cdot mCHr + 0.1241 \cdot m\,\mathrm{Pr}\,r \tag{G.11}$$

Therefore, the mass of the biogas and the digestate is calculated by Eqs.(G.12)-(G.13)

$$M_{biogas} = m_{CH4,digestor} + m_{CO2,digestor} + m_{NH3,biogas} + m_{H2O,biogas} \tag{G.12}$$

$$\begin{aligned} M_{digestate} = &(m_{lipids,feed} + m_{ch,feed} + m_{prot,feed}) \cdot 0.5 \\ &+ m_{rest,feed} + m_{NH3,digestate} + m_{H2O,digestate} \end{aligned} \tag{G.13}$$

However, it is necessary to determine the amount of H_2O and NH_3 in the liquid and gas phases. The rest of the gases are considered insoluble gases, following their Henry constants (Perry & Green, 1997). The thermodynamic equilibrium is used to establish the distribution of these compounds between the gas and liquid phases since most of the liquid phases consist of water and the amount of NH_3 dissolved in it is quite small. Thus, the laws of Dalton and Raoult (Eq.(G.14)) together with the concept of specific humidity are used to estimate the molar fraction of water (Eq.(G.15)) and NH_3 in both phases.

$$y_{NH_3,biogas} = Pv_{NH_3} \cdot x_{NH_3,digestate} \tag{G.14}$$

$$y_{H_2O,biogas} = \frac{MW_{H_2O}}{MW_{biogas-dry}} \cdot \frac{Pv_{H_2O}}{Pt_{Digestion} - Pv_{H_2O}} \tag{G.15}$$

The molecular weight of the dry biogas is calculated by Eq.((G.16)). The sum the molar fraction both liquid and gas phases must be 1 (Eqs (G.17) and (G.18))

$$MW_{biogas-dry} = \sum_i y_{i,biogas} \cdot MW_i \quad \forall i \in \{i = CH_4, CO_2, NH_3\} \tag{G.16}$$

$$\sum_i x_{i,digestate} = 1 \quad \forall i \in \{i = bat, lip, ch, prot, lig, ash, NH3, H2O, rest\} \tag{G.17}$$

$$\sum_i y_{i,biogas} = 1 \quad \forall i \in \{i = CH_4, CO_2, NH_3, H_2O\} \tag{G.18}$$

Through the molar fraction of the liquid and gas phases, it is possible to calculate the mass balances of water and NH_3 in both phases (Eqs.(G.19)-(G.22)).

$$m_{NH3,biogas} = y_{NH_3,biogas} \cdot N_{biogas} \cdot MW_{NH_3} \tag{G.19}$$

$$m_{NH3,digestate} = x_{NH_3,digestated} \cdot N_{digestate} \cdot MW_{NH_3} \tag{G.20}$$

$$m_{H_2O,biogas} = y_{H_2O,biogas} \cdot N_{biogas} \cdot MW_{H_2O} \tag{G.21}$$

$$m_{H_2O,digestate} = x_{H_2O,digestate} \cdot N_{digestate} \cdot MW_{H_2O} \tag{G.22}$$

Where N_{Biogas} and $N_{digestate}$ are the total moles of each phase. This variables are calculate through molecular weights of the chemical and Eqs.(G.23)-(G.24).

$$N_{biogas} = \sum_i \frac{m_{i,biogas}}{MW_i} \quad \forall i \in \{i = CH_4, CO_2, NH_3, H_2O\} \tag{G.23}$$

$$N_{digestate} = \sum_i \frac{m_{i,digestate}}{MW_i} \quad \forall i \in \{i = bat, lip, ch, prot, lig, ash, NH3, H2O, rest\} \tag{G.24}$$

It is now possible to estimate the volume of biogas, assuming that it behaves as an ideal gas following Eq.(G.25).

$$V_{biogas} = \frac{0.082 \frac{atm \cdot l}{mol \cdot k} \cdot 310K \cdot (\sum_i \frac{m_{i,biogas}}{MW_i}) \quad \forall i \in \{i = CH_4, CO_2, NH_3, H_2O\}}{Pt_{Digestion}} \tag{G.25}$$

To estimate the composition of the digestated, it is necessary to calculate the mass of carbon, organic nitrogen, NH_3, phosphorus, potassium, water, and the rest fraction. To do this, Eqs(G.26)-(G.33) and the initial composition of the waste (see Table G.3) are used.

$$m_{C,digestate} = f_{C,waste} \cdot f_{TS} \cdot m_{waste,feed}$$
$$-m_{CH_4,biogas} \cdot \frac{MW_C}{MW_{CH_4}} - m_{CO_2,biogas} \cdot \frac{MW_C}{MW_{CO_2}} \quad \text{(G.26)}$$

$$m_{_{Norg},digestate} = f_{Norg} \cdot f_{TS} \cdot m_{waste,feed} \quad \text{(G.27)}$$

$$m_{_{Nam},digestate} = f_{Nam} \cdot f_{TS} \cdot m_{waste,feed} - m_{_{NH3},biogas} \cdot \frac{MW_N}{MW_{NH3}} \quad \text{(G.28)}$$

$$m_{P,digestate} = f_P \cdot f_{TS} \cdot m_{waste,feed} \quad \text{(G.29)}$$

$$m_{K,digestate} = f_K \cdot f_{TS} \cdot m_{waste,feed} \quad \text{(G.30)}$$

$$m_{_{REST},digestate} = m_{_{REST},feed} = f_{REST} \cdot f_{TS} \cdot m_{waste,feed} \quad \text{(G.31)}$$

$$m_{H2O,digestate} = m_{H2O,feed} - N_{biogas} \cdot y_{H_2O,biogas} \cdot MW_{H_2O} \quad \text{(G.32)}$$

It is necessary to calculate the heat reaction of the digestion to estimate the amount of steam that has to be used to maintain the temperature of the reaction, that is, 37ºC. To do this, heat of combustion of chemical involved ($AH_{comb(i)}$) in the reaction (see Table G.1), together with the Eqs.(G.33), and (G.2) are used.

Table G.1: Heat of combustion for the chemical of a anaerobic digestion process

Chemical	Heat of combustion (kJ/g)
Ch	-18
Li	-13
Pr	-38
CH4	-50
SH2	-14.38
Biomass	-23.89
NH3	-18.64

$$Q_{digestion} = \sum_i AH_{comb(i)} \cdot (m_{i,biogas} + m_{i,digestate} - (m_{i,feed})) \qquad \forall i \in \{CH4, H2S, NH3, Biomass\} \tag{G.33}$$

Biogas upgrading starts with the removal of H_2S. For this purpose, an iron oxide bed is used since the temperature of the system is 37ºC and FeO works better than ZnO at this temperature (Sánchez et al., 2019). The reaction yield is 100%. A PSA system is used to remove the CO_2, NH_3, and H_2O present in the biogas. The system operates at 25ªC and 4.5 bar with a packed bed of zeolite 5A, which has an adsorption performance of 100% for NH_3, H_2O, and 95% for CO_2. Its selectivity to the rest of the components can be considered negligible (Erick León, 2016). The digestate is dehydrated through the use of a filter and stored (Taifouris & Martín, 2018).

G.1.2 *Modeling of gasification process*

Following the results of Sánchez et al., 2019, the type of gasification that provides the best economic performance for the transformation of waste into syngas is indirect gasification. This system is composed of a gasifier and a combustor (see Figure 9.1 of the manuscript). The energy exchange is carried out by a sand (olivine) that is fed at a ratio of 27 kg per kg of dry biomass. Gasification requires 0.4 kg of steam per kilogram of dry biomass (Sánchez et al., 2019). The heat required for gasification is generated by the combustion of the char produced in gasification. Therefore, it is an energetically self-sustaining system. The gasification is carried out at 1.6 bar (Sánchez et al., 2019), while the temperature of the process is a variable and sets the composition of the syngas. In fact, correlations that depend on the process temperature are used to determine the composition. The mole fraction of each component in the synthesis gas formed is estimated by Eqs.(G.34)-(G.40).

$$fmol_{CO,syngas} = 133.46 - 0.1029 \cdot T_{syngas} + 0.000028792 \cdot T_{syngas}{}^2 \tag{G.34}$$

$$fmol_{CO_2,syngas} = -9.5251 + 0.037889 \cdot T_{syngas} - 0.000014927 \cdot T_{syngas}{}^2 \tag{G.35}$$

$$fmol_{CH_4,syngas} = -13.82 + 0.044179 \cdot T_{syngas} - 0.000046467 \cdot T_{syngas}{}^2 \tag{G.36}$$

$$fmol_{C_2H_4,syngas} = -38.258 + 0.058435 \cdot T_{syngas} - 0.000019868 \cdot T_{syngas}{}^2 \tag{G.37}$$

$$fmol_{C_2H_6,syngas} = 11.114 - 0.011667 \cdot T_{syngas} + 0.000003064 \cdot T_{syngas}{}^2 \tag{G.38}$$

$$fmol_{H_2,syngas} = 17.996 - 0.026448 T_{syngas} + 0.00001893 \cdot T_{syngas}{}^2 \tag{G.39}$$

$$fmol_{C_2H_2,syngas} = -4.3114 + 0.0054499 \cdot T_{syngas} - 0.000001561 \cdot T_{syngas}{}^2 \tag{G.40}$$

The amount of syngas produced as well as tar also depends on the gasification temperature and can be calculated following Eq. (G.41) and Eq.(G.42) respectively.

$$mDrySyngas = 28.993 - 0.043325 \cdot T_{syngas} - 0.000020966 \cdot T_{syngas}{}^2 \tag{G.41}$$

$$mTar = 0.045494 - 0.000019759 \cdot T_{syngas} \tag{G.42}$$

6.6 % of nitrogen present in the lignocellulosic waste, as well as 8.3 % oxygen and 4 % of sulfur are retained by the char formed in the gasification process (Sánchez et al., 2019). The amount of carbon in the char is determined from the mass balances carried out at the gasification reaction. The amount of char is the sum of these 4 components.

The combustor is fed with 20 % excess air, preheated to 473K, and the char, which has a heat of combustion of 25000 kJ/kg (Blasi, 2004), provides heat to the olivine, which in turn will transfer it to the gasification process. To establish the amount and composition of the flue gases, as well as the heat generated in the process and the final temperature, mass and energy balances are carried out. In addition, the amount of Olivine that is lost with the syngas that has passed through the cyclones is added. Cyclones are used to separate the char, ash, and olivine from the syngas produced and flue gases, with an efficiency of 99.99% for the three compounds. To further reduce the amount of these three components in the syngas, two cyclones are placed in series. Finally, filter efficiency is used to complete the removal of char and olivine, prior to syngas upgrading and an electrostatic precipitator (99.99%) is used to purify the flue gas (Sánchez et al., 2019).

In order to use the syngas to produce biomethane, it is necessary to go through 3 stages of syngas upgrading. Steam reforming to transform all hydrocarbons to hydrogen, adsorption of H_2S using a FeO bed and a WGSR to adjust the H_2/CO_2 ratio to produce CH_4.

Following the techno-economic studies of Sánchez et al., 2019, among the two possible options to transform hydrocarbons to hydrogen, steam methane reforming is selected. The necessary heat is supplied by a fire heater fed by a part of the lignocellulosic residues. In the steam reforming process, while C_2H_6,C_2H_4 and C_2H_2 are fully converted to H_2 and CO, the amount of reacting methane is controlled by two thermodynamic equilibrium. These equilibrium are controlled by the equilibrium constants (kp1 for methane consumption and kp2 for water gas shift reaction), which depend on temperature, as shown in Eq.(G.43)-(G.44) (Sánchez et al., 2019).

$$kp1 = 10^{\left(-\frac{11650}{T(K)}+13.076\right)} = \frac{P_{CO}\ P_{H_2}^3}{P_{CH_4} P_{H_2O}} \tag{G.43}$$

$$kp2 = 10^{\left(-\frac{1910}{T(K)}-1.784\right)} = \frac{P_{CO_2} P_{H_2}}{P_{CO} P_{H_2O}} \tag{G.44}$$

By setting the equilibrium temperature, the partial pressures of each of the components that formed the gas are established, and the mass balances corresponding to the reformer are determined. In addition, the molar ratio between the steam used and the methane must be at most 20 and the temperature has a maximum value of 1600K. The bed of iron is designed to remove the SH_2 content in the syngas, with a conversion of 100% (Sánchez et al., 2019).

Once the hydrocarbons have been transformed into H_2 and CO, a WGSR is used to adjust the H2/CO ratio to an optimal value to maximize the production of biomethane and minimize the amount of H_2. For the mass balances of this reactor, Eq.(G.43)-(G.44) are used again, since the reactions involved are the same, and the temperature is adjusted to achieve the purpose shown above. In the methanation reactor, hydrogen and CO are used to produce CH_4 shifting the thermodynamic equilibrium (Eq.(G.43)) toward methane formation. The aim is not only to produce methane but also to consume as much of the hydrogen and CO as possible since they have to be removed from the biomethane so that it can be injected into the pipeline. The methanation reactor (MR) works at a pressure of approximately 23 bar (Sánchez et al., 2019). When this gas is expanded to

4.5 bar, the drop in temperature causes most of the water it contained to condense. The amount condensed is determined using the thermodynamic properties of saturated water vapor, as well as the concepts of absolute and relative humidity of the air (Eq.(G.45)).

$$specificHum = \frac{MW_{H_2O}}{MW_{biodry}} \cdot \frac{Pv_{H_2O}}{Pt_{PSA} - Pvt_{H_2O}} \tag{G.45}$$

For this it is necessary to determine the saturation pressure of the water, using Antoine's equation.

$$Pv_{H_2O} = 10^{\frac{A-B}{C+T(K)}} \tag{G.46}$$

To determine the molecular weight of the dry gas (Eq.(G.47)), it is only necessary to determine the mole fraction of each of the components without considering the water (Eq.(G.48)). In this way, the amount of water that biomethane can store can be determined, and by the difference with the total, the amount that condenses can be determined.

$$MW_{biodry} = \sum_j MW_j \cdot y_{dry_j} \tag{G.47}$$

$$y_{dry_j} = \frac{m_{j,MR}}{M_{MR} - m_{H2O,MR}} \quad \forall j \in [CH_4, CO, CO_2, H_2] \tag{G.48}$$

Once most of the water has been condensed by the temperature change, the stream is passed through a PSA tower, which similarly to the biogas purification process has efficiencies of 100% for H_2O and CO; and 95% for CO_2. Operating conditions are 25°C and 4.5 Bars (Erick León, 2016).

G.1.3 *Composition and production of waste and natural gas consumption in Spain*

In order to determine the manure production from the animal census, it is necessary to know the manure production by type of animal (Merino, 2006), the animal census (Instituto Nacional de Estadística, 2021), and the age distribution of the animal (Gobierno de España, 2022). For the case of Spain, these data can be consulted in Table G.2.

Both MSW and Sludge are estimated from the number of inhabitants, only in those cities with more than 50,000 inhabitants. It has been estimated that each person can produce 388 kg/year of MSW (INE, 2019) and 26.31

Table G.2: Manure production and ages distribution of the cattle in Spain

	Manure(tm/año)	Distribution
Cow	22	42%
Yearling (2+)	22	8%
Yearling (1-2 years)	19	13%
Calves (below 1 year)	11	37%

Kg/year of sludge(dried matter) (Bianchini et al., 2016) in Spain. Regarding lignocellulosic waste production, the crop production of Spain (Ministerio de Agricultura pesca y alimentación, 2019) together with the residue yield per type of crops (García-Condado et al., 2019) are used to estimate its production.

The composition of the residues is shown in Table G.3, for wet waste, and Table G.4 for lignocellulosic waste.

Table G.3: Composition of the wet wastes (Alibardi & Cossu, 2015; Nielfa et al., 2015; Kafle & Chen, 2016; Park et al., 2016; Li et al., 2021; Liew et al., 2022)

(Ts:Total solids)

	Manure(g/kgTS)	MSW(g/kgTS)	Sludge(g/kgTS)
Lipids	4.00	10.72	1.96
Carbohydrates	79.25	276.90	12.10
Protein	14.54	98.14	16.80
Total solids	22.00	14.00	17.00
Volatile solids	20.46	9.38	9.35
Total N	1.04	8.27	0.85
Organic N	0.52	0.44	0.25
Phosphorous	0.44	1.21	0.73
Potasium	2.81	4.43	3.65

Nevertheless, the estimation of the waste produced in each agricultural district can be carried out, in the case of the consumption of natural gas is not possible. The reports used to calculate the natural gas consumption (Comisión nacional de los mercados y la competencia, 2020) provide this information per province. This is not a problem for the methodology, since it only has to calculate the demand satisfied per province instead of per agricultural district, summing the contribution of each agricultural district

Table G.4: Composition of the lignocellulosic waste (Wilen et al., 1996)

	Elemental composition of the dried biomass
C	1.00
H	1.47
N	0.01
S	8.36E-4
O	0.66

that forms each province. In addition, methane consumption presented in these reports has energy units (i.e. GWh or BTU). However, for the methodology shown in this work, it is necessary to have this data in tons per year. For these, conversion factors based on the calorific value of natural gas can be used. The conversion factor is 13.1 kWh/kg (Boundy et al., 2011). The technical specifications, that the biomethane obtained must comply, with are shown in Table G.5.

Table G.5: Technical specifications of biomethane (Ministerio para la Transción Ecológica, 2018)

Chemical	Unit	Minimum	Maximum
CH4	mol %	90	
CO	mol %	–	2
H2	mol %	–	5
Fluorine	mg/m3	-	10
Chlorine	mg/m3	-	1
Amonia	mg/m3	–	3
Mercury	μg/m3	–	1
Siloxanes	mg/m3	–	10
Benzene, Toluene, Xylene(BTX).	mg/m3	–	500
Microorganism		0	0
Dust/Particles		0	0

G.1.4 *Design of the waste treatment plants/scale up*

Up to 50 different waste treatment plant designs are made for each type of waste following the mathematical models explained in the manuscript.

For facilities using anaerobic digestion as a waste treatment method, the maximum size of each plant must be limited in order to use the correlations in the literature to estimate the cost of the equipment (Couper et al., 2004). The maximum capacity will be fixed using measured values of usual capacities in this type of plant (Rico, 2020). This capacity is given in energy production values. Therefore, the amount of waste necessary to produce that electric energy per year is different for each type of waste (manure, MSW, and sludge), depending on their biogas production yields (see Table 9.4). In contrast, the minimum capacity is set by the minimum amount of waste generated in a county, provided that the waste is produced.

In the case of facilities that use gasification, the maximum and minimum capacity are fixed according to the maximum and minimum amount of waste generation per region considering the whole territory of Spain. In this case, it is not necessary to limit the maximum size because the correlations used for cost estimation can be applied for equipment sizes between those necessary to treat the maximum and minimum amount of waste considered. To determine the investment and the operating costs of the different designs, the procedure described in Sinnot, 2005 is used.

The correlations shown in the works of (Sánchez et al., 2019) and (Martín & Grossmann, 2011), as well as those published in (Couper et al., 2004), are used for the economic estimation of the following equipment.

Anaerobic digestion

PSA

This equipment is designed as a packaged vertical vessel. Based on this consideration, the cost estimate (Eqs.(G.59)) is given by calculating the amount of zeolite (Eqs.(G.49)-Eqs.(G.54)) and the size of the vessel (Eqs.(G.55)-(G.58)).

$$Mzeo = \frac{1}{q \cdot 0.65} \cdot \frac{(m_{CO2,PSAout} - m_{CO2,PSAin}) \cdot 1000}{MW_{CO2}} \cdot \eta \cdot \tau \tag{G.49}$$

$$q = \frac{qm \cdot K \cdot P_{CO2}}{1 + K \cdot P_{CO2}} \tag{G.50}$$

Where qm and K are calculated by Eqs.(G.51) and (G.52) (Martín-Hernández et al., 2020) , and P_{CO2} by Eq.(G.53)-(G.54) (Taifouris et al., 2021). The density of the bed (p_{zeo}) is 40 lb / ft (Sigma-Aldrich, 2022), the adsorption yield (η) is 0.95, the operation time (τ) is 20 min (Hauchhum & Mahanta, 2014) and the thickness of the equipment is calculated through Eq.(G.57)(Taifouris et al., 2021).

$$qm = -1.82355 \cdot 10^{-02} \cdot T(^{\circ}C) + 3.72021 \tag{G.51}$$

$$K = 1.63070 \cdot 10^{-03} \cdot T(^{o}C)^{2} - 3.68662 \cdot 10^{-01} \cdot T(^{o}C) + 27.3737 \tag{G.52}$$

$$P_{CO2} = y_{CO2} \cdot Pt_{PSA} \tag{G.53}$$

$$y_{CO2,PSA} = \frac{m_{CO2,MS3}}{M_{MS3}} + \frac{m_{CO2,Sep2}}{M_{Sep2}} \tag{G.54}$$

$$Vzeo = \frac{m_{zeo}}{\rho_{zeo}} \tag{G.55}$$

$$Dcads = \sqrt[3]{\frac{6 \cdot Vzeo \cdot \pi}{7}} \tag{G.56}$$

$$ecads = 0.023 + 0.003 \cdot Dcads \tag{G.57}$$

$$Whads = \rho_{steel} \cdot \ \pi * \left(\left(\frac{dcads}{2} + ecads \right)^{2} - \left(\frac{dcads}{2} \right)^{2} \right) \cdot \ 4 \ \cdot Dcads + \ \frac{4}{3} \cdot \pi \cdot \ \left(\left(\frac{dcads}{2} + ecads \right)^{3} - \left(\frac{dcads}{2} \right)^{3} \right) \tag{G.58}$$

$$\mathrm{Cos}\, t_{ads} = \left(\left(1.218 \cdot e^{8.571 - 0.2330 \cdot \log(Wads) + 0.04333 \cdot \log(Wads)^{2}} \cdot 1.7 + 1669 \cdot Dads^{0.2029} \right) \right) \cdot 2 + (Mzeo \cdot 5) \cdot 2 \tag{G.59}$$

The bed of iron

The bed of Fe to remove the H_2S is designed in a similar way to PSA, through the amount of Fe required. Therefore, the amount of Fe is estimated by Eq.(G.60) using stoichiometric ratios (1 g can remove 2.5 g of H_2S (Siefers et al., 2010)). Because of the reduced amount of H_2S present in the gas, the renewal period of the iron is set at 10 years. The density of the iron bed (ρ_{Fe}) is 644.24 kg/m^3 (Siefers et al., 2010). Next, the previous equations (Eqs.(G.56)- (G.59)) and Eq.(G.61) are used to estimate the cost of this equipment.

$$MFe = \frac{(m_{H2S,bioreactor}) \cdot 60min/h \cdot 24h/day \cdot 365Day/year \cdot 10year}{2.5gH_2S/gFe} \tag{G.60}$$

$$V_{Fe} = \frac{m_{Fe}}{\rho_{Fe}} \tag{G.61}$$

Digetors

Three possible digester sizes are established, 1000 m^3, 2000 m^3, and 3000 m^3, following the work of Taifouris and Martín, 2018. From these sizes, the costs are estimated following the equation (G.62)- (G.64).

$$Cost_{Small\ \ Bioreactor} = 17069 \cdot V_{Small\ \ Bioreactor}^{-0.551} \tag{G.62}$$

$$Cost_{Medium\ \ Bioreactor} = 17069 \cdot V_{Medium\ \ Bioreactor}^{-0.551} \tag{G.63}$$

$$Cost_{Large\ \ Bioreactor} = 17069 \cdot V_{Large\ \ Bioreactor}^{-0.551} \tag{G.64}$$

The total volume processed in the waste treatment plant depends on the number of reactors installed and the type of reactor. Therefore, the total capacity of the bioreactors is calculated by Eq.(G.65).

$$CapTBio = Nm_{Small\ \ Bioreactor} \cdot V_{Small\ \ Bioreactor} + \\ Nm_{medium\ \ Bioreactor} \cdot V_{medium\ \ Bioreactor} + Nm_{large\ \ Bioreactor} \cdot V_{large\ \ Bioreactor} \tag{G.65}$$

The volume of waste sent to the treatment plant in each 21-day cycle has to be less than the treatment capacity of the plant Eq.(G.66).

$$\frac{m_{waste,bioreactor}}{100} \cdot 60\frac{min}{h} \cdot 24\frac{h}{day} \cdot 21day \leq CapTBio \tag{G.66}$$

The total cost of all digesters is estimated by Eq.(G.67).

$$C_{bioreactor} = \sum_{z} Cr_z \cdot Nr_z \tag{G.67}$$

Compressors

The cost of the compressors is estimated from their power, following Eq.(G.68).

$$C_{compress} = 1000 \cdot 1.81 \cdot \left(W_{compres} \cdot 1.34\right)^{0.71} \tag{G.68}$$

Heat exchangers

To determine the cost of the heat exchangers, it is necessary to determine the heat exchange area. For this purpose, the Eq.(G.69) is used. The heat is determined through energy balances to the waste treatment process.

$$Q_{ex} = U \cdot LMTD_{ex} \cdot A_{ex} \tag{G.69}$$

The logarithmic mean temperature (LMTD) is determined by the Eq.(G.70) and the global coefficient of heat transfer (U) can be consulted in Sinnot, 2005.

$$LMTD = \frac{\Delta T1 - \Delta T2}{\log\left(\frac{\Delta T1}{\Delta T2}\right)} \tag{G.70}$$

Once the area has been determined, the cost is calculated following Eq.(G.71)

$$\begin{aligned} Cost_{exc} = 1.218 \cdot \left(e^{1.1156+0.0906 \cdot \log A_{exc}}\right) \cdot \\ \left(e^{8.821-0.30863 \cdot \log A_{exc}+0.0681 \cdot \log A_{exc}{}^{2}}\right) \end{aligned} \tag{G.71}$$

Gasification process

Fire heater

The cost of the fire heater is estimated from the heat required for the reforming process, that is, the heat generated in this equipment, following Eq.(G.72).

$$Cost_{FireHeater} = 1.218 \cdot 25.5 \cdot Q_{\mathrm{Re}\,form}^{0.86} \tag{G.72}$$

Gasifier

The cost of the gasifier is related to the amount of waste, as indicated by Eq.(G.73).

$$Cost_{gasifier} = \left(\frac{16.3 \cdot m_{waste,feed} \cdot MW_{waste} \cdot 3600 \cdot 1000}{68.8}\right)^{0.65} \tag{G.73}$$

Cyclon, precipited electrolizer and filter

The cost of the cyclones depends on the volume of gas treated (Eq.(G.74)), as do the electrostatic precipitator and filter (Eq.(G.75)-(G.77)). However, in the case of the electrostatic precipitator, if the plant capacity is less than 0.5 kmols/s, Eq.(G.75) is used, otherwise Eq.(G.76) (Industries, 2022).

$$C_{Cyclon} = \left(4.463 \cdot V_{Cyclon}\right) \tag{G.74}$$

$$C_{Ep} = (5111.6 \cdot V_{elect} + 149832) \tag{G.75}$$

$$C_{Ep} = (10549 + 1.75 \cdot Velect) \tag{G.76}$$

$$C_{Filter} = (5497.4 \cdot V_{Filter}) \tag{G.77}$$

Reformer, WGSR, metanador and bed of ZnO.

The costs of this equipment are estimated similarly to the PSA system and the iron bed. First, the amount of catalyst required for the reaction/adsorption (Eq.(G.78)) is determined. Then, the volume of the reactor is determined, using the gas hourly space velocity (GHSV) Eq.(G.79). The values of GHSV for the different equipment can be seen in Table G.6.

Table G.6: GHSV for the different processes considered (Sánchez et al., 2019)

	GHSV($\mathbf{h^{-1}}$)
Steam Reforming	5000
WGSR	4000
Methanation	8000

To determine the diameter, thickness, and weight, the Eq.(G.56)-(G.58) presented above are used since these devices are also designed as packaged vessels. For cost, the equation Eq.(G.59) is used. GHSV and density and catalyst density can be consulted in the works of Sánchez et al., 2019

$$Mcat_{\text{Reform}} = \frac{\sum_{j} \frac{m_{\text{j,Reform}} \cdot R \cdot T_{\text{Reform}}}{MWj \cdot P_{\text{Reform}}} \cdot 3600 \frac{s}{h} \cdot \rho_{cat}}{GHSV_{reform}} \tag{G.78}$$

$$V_{\text{Reform}} = \frac{\sum_{j} \frac{m_{\text{j,Reform}} \cdot R \cdot T_{\text{Reform}}}{MWj \cdot P_{\text{Reform}}}}{GHSV_{reform}} \tag{G.79}$$

Update of equipment prices

The prices of each of the equipment are updated using CEPCI values, that can be consulted in the literature (Engineering, 2022). In addition, the currency is updated, changing prices and costs from the US dollar (currency used in the cost correlations of the references consulted) to the euro (Investing, 2022).

Total investment cost and operating cost of factories

The purchase cost of major equipment items (PCE) is calculated by adding the cost of each of equipment. Eq.(G.80) is used to estimate the PCE of the gasification plant, while Eq.(G.81) calculates the PCE of the anaerobic digestion plant.

$$\begin{aligned} PCE_{Gas} &= Cost_{Fh} + Cost_{Gasr} + Cost_{Cyclons} + Cost_{Ep} \\ &+ Cost_{Filter} + Cost_{Exs} + Cost_{Comps} + Cost_{Met} + Cost_{WGSR} + Cost_{\mathrm{Reform}} \end{aligned} \tag{G.80}$$

$$PCE_{Dig} = Cost_{PSA} + Cost_{Fe} + Cost_{Dig} + Cost_{Comps} + Cost_{Exs} \tag{G.81}$$

In addition to the equipment cost, it is necessary to consider other additional costs to determine the physical plant cost (PPC) (Eq.(G.82)), which are shown in Table G.7. The fixed capital (FC) is estimated considering the factors of f7, f8, and f9. Finally, the total investment cost (TIC) is determined by adding 5% (Eq.(G.84)) to the FC.

$$PPC = PCE \cdot (1 + f1 + f2 + f3 + f4 + f5 + f6 + f6) \tag{G.82}$$

$$FC = PPC \cdot (1 + f7 + f8 + f9) \tag{G.83}$$

$$TIC = FC \cdot 1.05 \tag{G.84}$$

Operating costs (OC) are composed of variable costs (VC) and fixed costs (FC) (Eq.(G.85)). VC correspond to the sum (Eq.(G.86)) raw materials (RM) (Eq.(G.87)) and auxiliary services (Aux) (Eq.(G.88)), while FC are maintenance (Ma), labor (La), depreciation (Cc), plant overhead (Po), laboratories (Lab) and insurance (In) (Eq.(G.89)).

$$OC = VC + FC \tag{G.85}$$

Table G.7: Factors for estimation of project PPC and FC

Item	Description	value
f1	Equipment erection	0.45
f2	Piping	0.45
f3	Instrumentation	0.15
f4	Electrical	0.1
f5	Buildings, process	0.1
f6	Utilities	0.45
f7	Storages	0.2
f8	Site development	0.05
f9	Ancillary buildings	0.2
f10	Design and Engineering	0.25
f11	Contractor's fee	0.05
f12	Contingency	0.1

$$VC = RM + Aux \tag{G.86}$$

$$RM = WaterP + M_{olivine} \tag{G.87}$$

$$Auxiliary = TotalPower + WaterA + Steam \tag{G.88}$$

$$FC = Ma + La + Po + Lab + Cc + In = 0.05 \cdot FC + 5 \cdot 3 \cdot 24 \cdot 365 \cdot 24 \cdot 2 + 0.5 \cdot OC + 0.3 \cdot OC + 0.06 \cdot FC + 0.01 \cdot FC \tag{G.89}$$

G.2 SCALE-UP AND DIFFERENT DESIGNS OF WASTE TREATMENT

After analyzing the waste generation in each of the regions considered in the case of Spain (see Figure 9.3), the minimum and maximum capacities of the treatment plants for each of the wastes considered are established. In this way, 50 designs with different processing capacities are carried out following the indications described in Section G.1.4. The results of sizing, OPEX and COPEX of each design can be consulted in Figures G.1-G.3. To determine the amount of methane produced by each plant, its waste treatment capacity and the yields shown in Table 9.4.

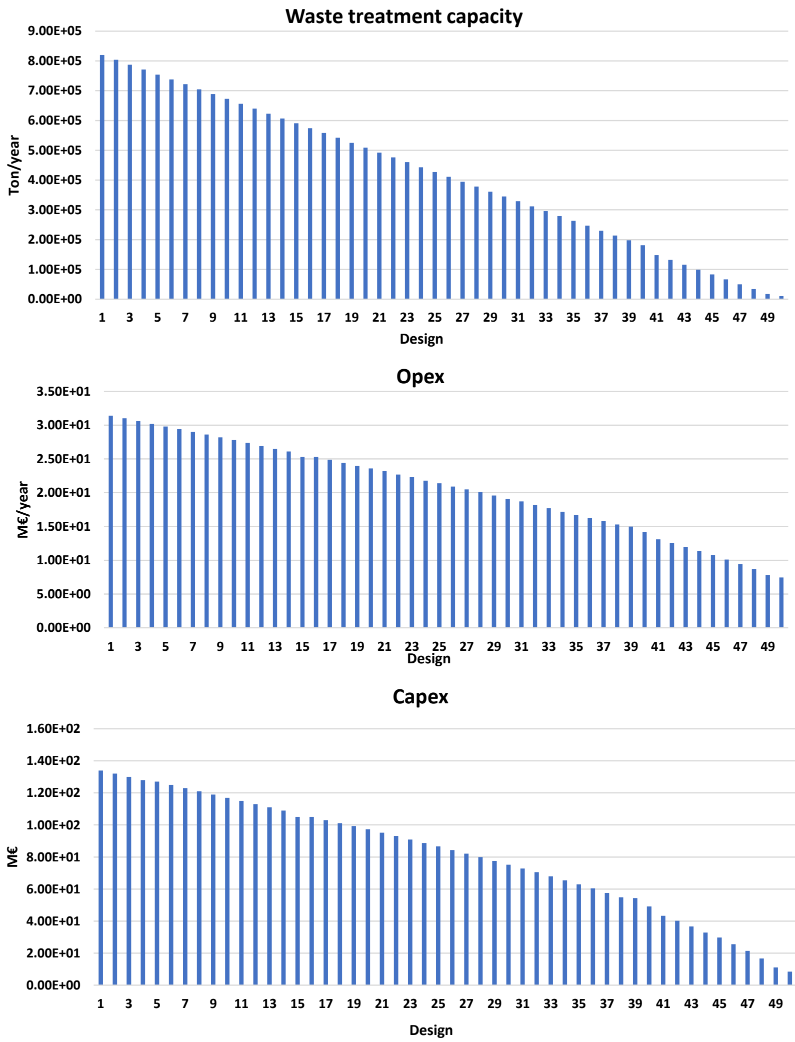

Figure G.1: Capacity, OPEX and COPEX of the different design of lignocellulosic waste treatment plants

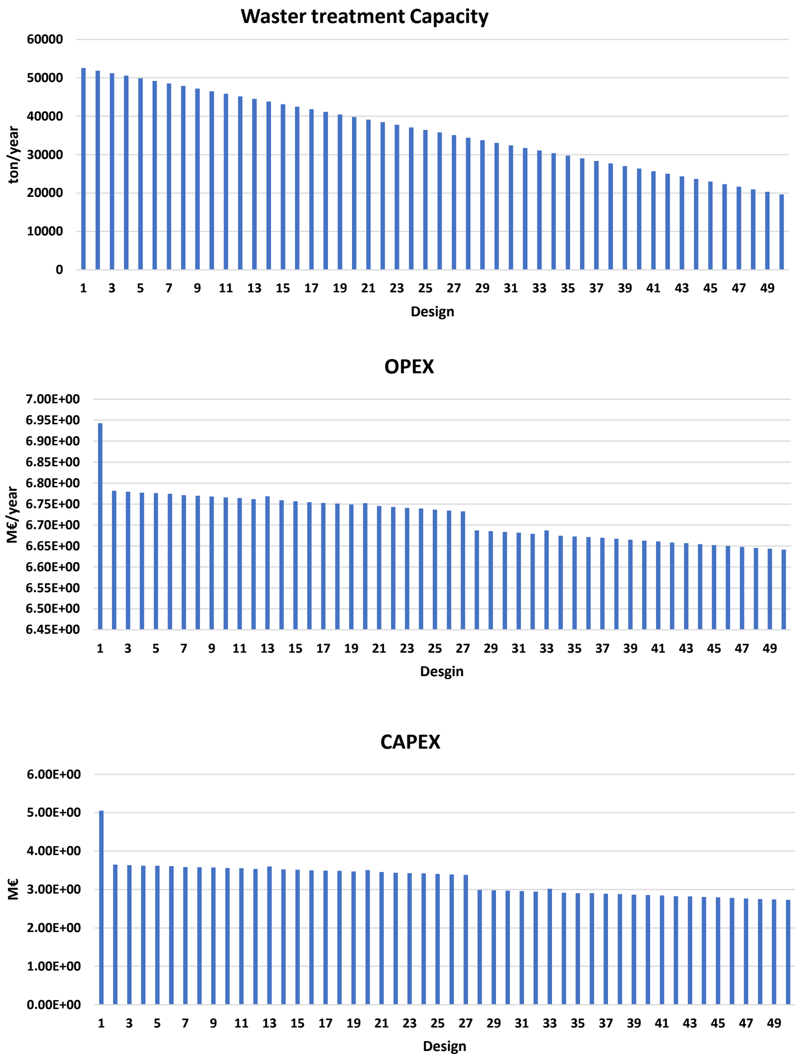

Figure G.2: Capacity, OPEX and COPEX of the different design of msw treatment plants

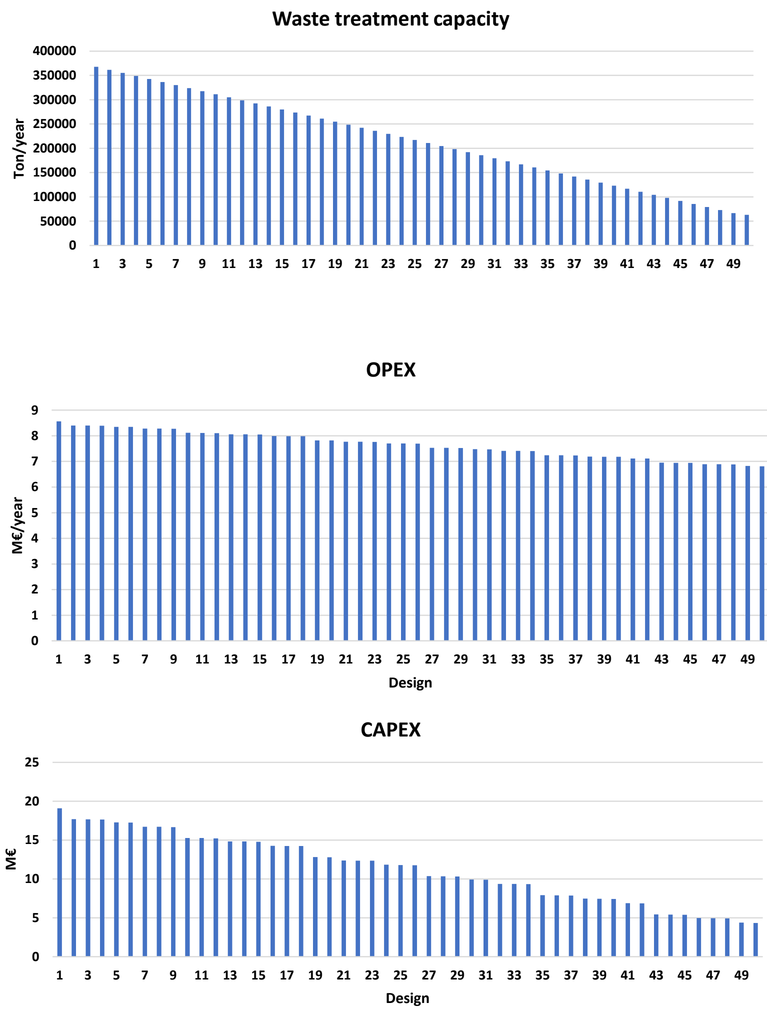

Figure G.3: Capacity, OPEX and COPEX of the different design of manure treatment plants

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