Appendix A:

Exergy in industrial ecology

This work makes extensive use of exergy as the main measurement unit for the magnitudes that are used throughout it. That is why in this section the details about exergy are explained, its purpose, its uses, and how to calculate it, all from the point of view of the discipline that uses it in this way, that is, industrial ecology. In order to better understand it, a small synopsis of the thermodynamics concepts and formulations needed to do so is also developed.

A.1. Introduction

In the field of industrial ecology it is very important the accounting of the flows and their evaluation. Material flow analysis (MFA) and input-output traditional analysis use monetary units (€, $...) o physical units, that can be of mass (kg, t), energy (MJ, kWh...), etc.

Accounting the flows in terms of monetary units has the inconvenience of being partially arbitrary, since they depend on exterior elements as markets or currency speculation. Moreover, monetary indicators don't represent universal values that can be understood by everyone. It isn't the same to account in euros that in dollars, for example. Nonetheless they have the advantage of allowing all the flows to be measured in the same unit. Also, monitary indicators permit to aggregate and disaggregate the results according to the scope of the study.

A rigorous, universal analysis must be presented in a physical quantity, though. A kilogram of iron or a 100 kWh of natural gas give the same information in whichever part of the world. Besides, information is independent of any exterior economical factor, and won't be affected by inflation or currency fluctuation. Regardless, the vast majority of physical indicators have an important problem: each substance to analyze will require a different measurement unit. This fact creates another difficulty, the impossibility of aggregating and disaggregating results. We cannot add quantities of mass to those of energy for example.

A way to maintain objectivity and universality of indicators while keeping the possibility of aggregating and disaggregating results, comes from the concept of “exergy”

A simple way to describe exergy is as a physical measure of the quality of a system in energetic terms. All substances can be measured in exergy using the same unit (Jules, for example) and, consequently, the results are easily compared and can be aggregated or disaggregated at will. Exergy puts together in one indicator all the physical properties of a resource employed in a process and simplifies greatly the analysis.

The main drawback of exergy is that, being a magnitude known mostly in academic circles, is not widely known by administrators.

We will now go through a small review of the thermodynamics concepts on how to calculate exergy and its physical meaning.

A.2. Basic thermodynamics

To be able to fully understand the meaning and calculation process of exergy, we will have first to go quickly over the first and second laws of thermodynamics.

A.2.1. The first law of thermodynamics

The first law of thermodynamics, or energy conservation law, is the general principle of physics. It can be enunciated in several ways, but all of them have essentially the same meaning: energy is always conserved. Some of the most used definitions are:

-When energy is transformed from one form of energy to another the amount of energy is maintained.

-Energy cannot be created nor destroyed.

-The total sum of energies is constant.

-The net work done to a closed system in an adiabatic process depends only on the initial and final points, not the details of the process.

The magnitude we use when using the first law is energy [J]. There are three ways in which energy is usually treated. internal energy (U), related to the positions, internal state and movements of the atoms of a substance; potential energy (E_p), related to the position of a substance in a system; and kinetic energy (E_k), related to the movement of a system.

The energy of a system is the sum of those forms of energy

$$E=U+E_p+E_k$$

And the balance of energy in a system is calculated as:

$$\Delta E=Q-W$$

Where Q is the heat entering a system and W the work exiting it. That means that there are only two ways of energy in movement: work and heat.

When changing something that alters the equilibrium of a system, it will evolve to another state of equilibrium, and in the process it will have exchange only heat and/or work.

The usefulness of this law comes from the fact that, being an expression of equivalence, it allows to spare complicated measures of the flows coming in and out of a system. If we have the information about two out of three flows, we won't need to measure the third, as it is value can be obtained through the balance above.

A.2.2. The second law of thermodynamics

There are also several ways of expressing the second law of thermodynamics, depending mostly on the person who enunciated it. As done in the previous case, here are two of the most common:

-Clausius statement: No process is possible whose sole result is the transfer of heat from a body of lower temperature to a body of higher temperature.

-Kelvin statement: No process is possible in which the sole result is the absorption of heat from a reservoir and its complete conversion into work.

One of the most used ways to enunciate this principle, though, is that the entropy of an isolated system never decreases, or to put it another way, everything evolves naturally to its state of maximum degradation.

The property associated to this law is entropy (S). This magnitude relates heat with temperature, being its unit J/K. It's also a measure of the state of disorder of a system.

The entropy balance of a system is calculated as follows:

$$S_2 - S_1 = \int_1^2 \left(\frac{\delta Q}{T} \right) + \sigma$$

Where σ represents the irreversibilities of the process.

In any process, the entropy of the system plus that of the environment will always increase, or be maintained equal at the very least. Therefor, if every process implies a degradation and energy is always maintained, there will be forms of energy more degraded than others, being thermic energy the final state of every form of energy.

A.3. Exergy

The combination of the first and second laws indicates that energy will only be transformed if its quality is decreased, since the first law states that the amount of energy will not change and the second law says that it will be transformed into a more degraded state. We call that quality of the energy, exergy.

Exergy is a thermodynamic magnitude that indicates the maximum amount of work that can be extracted from a system by spontaneous interaction of that system with its environment. It also indicates the minimum amount of work that has to be given to the system to take it back to its original state. When a system reaches equilibrium with its environment, we say that has reached “dead state”.

It ts exergy the reason why, for example, we would always choose energy in form of electricity over the same amount of thermic energy. It is easy to transform electricity into heat and we can do it completely, but the opposite is not true, obtaining electricity from heat is more difficult and the transformation will never be complete. The same could be said about concentrations, we would no doubt choose copper in a mine over that in the earth surface, that, being much less concentrated, would require huge amounts of energy in order to be extracted.

All materials have a defined and calculable amount of exergy in relation to a referential environment. Exergy is an extensive magnitude with the same units that energy and, therefore, is a universal property that:

-Can never be negative.

-It isn't conserved, but destroyed by irreversibilities.

-Always have losses in material or energy transformations.

Kinetic, potential, magnetic and electric exergies equal the respective energies. When calculating exergy for heat flows, it can be expressed as:

$$B = Q \frac{(T - T_0)}{T}$$

Where T is the temperature of the flow and T_0 is the temperature of the environment

According to this formula, we can see that exergy can never be negative, because when the temperature of the flow is greater than that of the environment, then the heat is positive, while when temperature is lower than that of the environment, the heat is negative and exergy comes out positive again.

To calculate chemical exergies we need to establish a referential environment. Several environments have been proposed. Perhaps the most widely used is the one proposed by J. Szargut and can be assimilated to a thermodynamiclly dead planet, where all materials have exhausted their possible chemical reactions and have been dispersed and mixed. This hypothetical environment has 85 substances of reference, each corresponding to one element. The final result is a table with the chemical exergy of each element, obtained through various geochemical approximations. This allows to calculate the exergy of a compound as the sum of the chemical exergy of its elements plus the gibs energy of the compound, that can also be looked up in tables.

The exergy of a flow is the sum of all the exergies contained in it.

A.4. Energetic and exergetic efficiency

The efficiency of a system is a measure of how well it is performing its function, that is, how many resources it needs to fulfil its purpose. Given an established function to be performed by the system, the less resources it spend to do it the better its efficiency will be. Mathematically, the efficiency is usually defined as the ratio between the net work coming out of a system (W) and the heat coming into the system (Q).

$$\eta=\frac{W}{Q}$$

There is a limit, though, to that efficiency when defined as above. The maximum efficiency that can be achieved that way is performed by a Carnot cycle, a theoretical thermodynamic cycle composed of two processes at constant temperature and two processes at constant entropy. That maximum efficiency that a system can reach is:

$$\eta_{max}=\frac{T_h-T_c}{T_c}$$

Where T_h is the temperature of the high temperature reservoir and T_c is the temperature of the low temperature reservoir.

But, efficiency as has been just shown, doesn't provide any information about the best possible operation by itself, if not compared with the maximum efficiency. Exergy efficiency, being based on the second law, overcomes that issue, since it differentiates between the use of energy resources that are, from a thermodynamic point of view, more efficient than others.

Exergy efficiency can be expressed as the ratio between the exergy provided by the system (B_o) and the one required by the system (B_i):

$$\varepsilon=\frac{B_o}{B_i}$$

Appendix B:

Input-output methodology

Input-output methodology or input-output analysis is a very useful tool when studying complex systems that exchange flows between them. Even if originally developed for economic systems, this methodology will be key for the purposes of this work, since it is the foundation of thermoeconomic input-output analysis, that will be introduced subsequently.

In this appendix we will shortly go through the concept of input-output methodology, its characteristics, input-output tables and matrix, and input-output cost calculation.

B.1. Input-output analysis description

Input-output methodology is being used more and more when it comes to the industrial ecology analysis of a system. One of its most useful characteristics is that it allows to study the variations of the internal flows of the system when exterior conditions change.

Input-output analysis studies the interdependences between industrial processes in an economic system. It was developed by Wassily Leontief at the end of the thirties and he received the Nobel Price of Economy in 1973. Since Leontief built the first input-output table, governments all around the world have been using them regularly. Now-a-days most of the countries of the world use this methodology to diagnose their economies.

Input-output analysis has become one of the most important statistical tools to so many countries due mainly to its simplicity and great capacity.

This methodology is applied on large fields of economics (including industrial ecology) to:

1) Quantitative evaluations of products, consumptions and environmental impact of an economic system.

2) Estimate the effect of the demand variation of a product, a process, or the change of a type of tecnology, over the production of the other components of the system.

3) Obtain the price/cost of products as a function of the price/cost of the resources of a system.

B.2. Characteristics

Generally, input-output analysis divides the system on a number of subsectors and consider the material, energy and (if suited) services getting in and out of the sector. Since each sector can have flows coming from and going to any other sector, the quantity of information contained in the model grows quickly when increasing the number of analyzed sectors.

In the case of industrial ecology, the sectors will be called processes. Each process is represented by a set of inputs (resources) that are used to obtain a set of outputs (products). The combination of processes related by their inputs and outputs creates the system. In turn, systems are determined by the processes that constitute them and their relations to their surroundings.

In general, processes are defined as “black boxes”, in the sense that the reactions or transformations that may occur within the process are of no relevance. Only the inputs and outputs of the processes are important.

In figure 1.1, in the main document, there is an example of the hypothetical input-output model of an economy. We can see the flows coming in and out of every sector, the inputs and outputs, and the flows going through the limit of the system, imports and exports.

The inputs and outputs of a process are proportional to the level of productivity, so if we double, for instance, the production of a good, the necessary resources and all of the intermediate flows that go through every analyzed process will be doubled too.

B.3. Input-output tables

Essentially, the basic form of an input-output table is represented by rows and columns. The rows are the outputs of a given sector, while columns indicate the destiny of the outputs. Therefore, the matrix represents an economic system of double entrance, where the sum of all the inputs equals the sum of all the outputs. The input-output table for figure 1.1 is shown below in figure B.1.

Sector	Government	Households	Intermediate s.	Capital	Final demand
Government			Public services		
Households			Labor		
Intermediate s.	Goods & services	Consumption goods		Investments	Exports
Capital			Capital consumption		

Figure B.1 Input-output table

For further clarification, figure 1.2, also in the main document, shows a numerical example of an input-output table. Each value within the central matrix represents the flow from the sector i to the sector j. That value is, logically, both the output from i to j and the input to j from i. Hence, the flow that goes from sector 3 to sector 2 is 82 and the one that goes from 2 to 3 is 11. Final demand and value added (also called external resources) are, respectively, the flows that go out and into the global system. For example, the sector 5 has an output to exterior of the system of 220 units, while the input from outside the system to sector 5 is 128. Total output/input is the sum of all the outgoing or incoming flows in a sector. The total input of sector 4 would be 432 in our example. It can also be observed that, as said before, the sum of all the inputs equals the sum of all the outputs.

B.4. Matrix analysis

It is possible to use the input-output table to create a create a matrix of coefficients that will be used to do the calculations of this method.

First we establish the total output (x_i) of every sector as the sum of the output to every other sector (x_{ij}) plus the output to the outside of the system (d_i).

$$x_i = d_i + \sum_{j=1}^{n} x_{ij}$$

To illustrate: The total output of sector 7 in our numerical example will be 561 (349+1+45+26+42+4+47+22+25)

Next we define the technical coefficients as the amount of output from *i* to *j* that *j* uses to produce one unit of its total output.

$$a_{ij} = \frac{x_{ij}}{x_j} ; A_{ij} = \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \dots & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix}$$

And now, using those coefficients, the total output of a sector can be expressed as:

$$x_i = d_i + \sum_{j=1}^{n} a_{ij} x_j$$

That can finally be expressed in a matrix formulation:

$$\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} a_{11} & .. & a_{1n} \\ \vdots & .. & \vdots \\ a_{n1} & .. & a_{nn} \end{pmatrix} * \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} d_1 \\ \vdots \\ d_n \end{pmatrix}$$

Working out the value of x_i:

$$\overline{x}=\left(U-A_{ij}\right)^{-1}\overline{d}$$

Where U is the identity matrix. And $\left(U-A_{ij}\right)^{-1}$ is known as the Leontief Matrix (L)

Wich is the expression we were looking for, as it allows to calculate the variations on the outputs of every sector when the demand (the exterior conditions) change.

The matrix of coefficients is always defined per unit of product. This is a great advantage, because it permits to make calculations independently of the total production of the system.

B.5. Obtaining of costs

Obtaining the costs of each sector of a system is key, both to its diagnosis, and its optimization. But also, in industrial ecology, plays a central role in establishing fair prices for the exchanged flows.

Usually, residues coming from industries are picked up by specialized companies that treat them and manage their disposal. These services can represent considerable expenses for the industries. If another company is interested in the residues of the first company as resources, it won't only solve the problem of the residues but could even be transformed into a source of income. Of course that rises the question of at what price the residues should be sold. This is one of the cases in which input-output analysis could be used to answer.

To calculate the cost of the flows of a system we assume that the cost of the inputs coming from outside the system are known. The production cost of each sector equals the sum of the costs of all its inputs. Using the a_{ij} coefficients seen before and expressing the costs of each sector as unitary production costs (c_i), we obtain the following formulation:

$$c_i=b_i+\sum_{j=1}^{n} a_{ji}c_j$$

Where b_i are the unitary cost of the exterior resources. Notice that the order of the a_{ij} coefficients is now inversed in relation to the formulation used previously for outputs.

Expressing this in matrix formulation:

$$\begin{pmatrix} c_1 \\ : \\ c_n \end{pmatrix}=\begin{pmatrix} a_{11} & .. & a_{n1} \\ : & .. & : \\ a_{1n} & .. & a_{nn} \end{pmatrix}*\begin{pmatrix} c_1 \\ : \\ c_n \end{pmatrix}+\begin{pmatrix} b_1 \\ : \\ b_n \end{pmatrix}$$

Working out c_i and putting it into a more compact notation:

$$\overline{c} = \left(U - A_{ij}^{T} \right)^{-1} \overline{b}$$

Which is the expression we were looking for, since it allows to calculate the cost of the flows out of the cost of the exterior flows.

Appendix C:
Thermoeconomic analysis

C.1. Definition of thermoeconomics

In a first approximation it would seem that economics and thermodynamics have little in common. The first is among the social sciences and studies the correct distribution of limited resources to satisfy the needs of human beings. The second one is related to physics and engineering and studies energy transformations. Nonetheless, if the subject is looked into for a while, similarities begin to come up.

To begin with, economics are related to the use and distribution of natural resources, both sources of energy and materials, since productive systems and technological development are dependent on them. Also, thermodynamics allow, through their first and second law, to quantify the amount of resources consumed in a given process.

In this context, thermoeconomics (Name proposed by Evans and Tribus in 1962) are based on the combination of thermodynamics (Second law) and economics (Concept of cost). This discipline was born in the seventies and its goal is to study the connexion between thermodynamics and economics, lay down the theoretic principles of a science for energy saving, and obtain this way models that express the limits of not having an unlimited amount of natural resources, looking for general criteria that allow to evaluate the efficiency and the cost of its products, in systems with a high energy consumption. Besides, since exergy is useful not only to quantify energy flows, but also material flows, thermoeconomics can be seen as a powerful tool to analyze flow aggregation, which is characteristic of industrial ecology.

Thermoeconomics give methods to evaluate the quantity and quality of material and energy losses, and to evaluate the cost of those losses in terms of natural resources (energy-based or otherwise). Along the years, in the field of thermoeconomics methods have been developed to:

-Rational establishment of prices based on physics criteria.
-Process optimization according to energy and material saving criteria.
-Process inefficiency detection and calculation of its impact on resource consmption.
-Process synthesis and integration, included those related to industrial symbiosis.

For reasons of space we will only focus on some basic aspects of thermoeconomic analysis. Because of this, the fundamental concepts of thermoeconomics will be introduced, avoiding an excess of mathematical formulations, even if those formulations are a key aspect of the methodology. Fortunately, cost calculation is very similar in a lot of situations to input-output analysis, as will be seen when the formulations aspects are introduced. The main difference appears as a result of the use of exergy as the variable to quantify all of the flows. This has two consequences:

-All of the flows are measured in the same magnitude, so they can all be compared.
-In each component or part of the system, exergy always decreases (second law)

C.2. Purpose and efficiency

The second law of thermodynamics establishes that the exergy entering a system will always be higher to the one coming out of it.

$$Incoming\_exergy - Outcoming\_exergy = Irreversibility$$

Where irreversibility is always > 0

A first approximation to quantify the quality of a process is to consider its irreversibility. In an ideal process, irreversibility would be zero, while in a real process it is always higher. This magnitude presents an inconvenience, as it doesn´t take into account the scale of the process. It is not the same to have an irreversibility of 10 kW in a small domestic heater than to have it in an industrial heat exchanger. To solve this, the quality of processes is measured through the concept of efficiency. This concept is older than thermodynamics and it is defined, as it is well known, as:

$$Efficiency = Product / Fuel$$

The former equation is very important for thermoeconomics, as it will be seen shortly. There are no inputs or outputs in it, only fuel and product. Consequently, it is necessary to define, for each component, its purpose (product), and the resources used to accomplish that purpose (fuel). This is only possible when the process has been designed with a given purpose. When product and fuel are expressed in exergy units, its value will variate between 0 and 1 (the last one being only possible in ideal processes). Once the purpose has been defined and expressed in exergy, the exergy balance can be written as follows:

$$Resources(F) - Product(P) = Irreversibility$$

This equation shows that, to produce a product (P), a certain amount of resources (F) are required, part of which are always lost due to irreversibility.

It is important to insist on the difference between input/output and fuel/product. Sometimes they can be equal, but this is not the usual situation. As it has been said, it depends on the purpose of the system. For instance, in a domestic heater natural gas is combusted to heat water, consequently, its fuel is the exergy of the gas, and its product, the exergy of the hot water minus the exergy of the cold water. In a heat exchanger, the hot flow gets colder (its exergy decreases) and the cold flow gets hotter (its exergy increases). In that situation, fuel is the loss of exergy of the hot flow, and the product, the gain of exergy of the cold flow. In a turbine of a thermic power plant, steam expands to produce work, so fuel es the exergy loss of the steam, and the product is the mechanical work.

C.3. Cost formation process

A basic concept in thermoeconomics is the idea of cost. As a general rule we can define the cost of something as the amount of resources that have been required to make it available Particularly, the exergetic cost of an exergy flow B, is the amount of exergy necessary to produce it, and it is represented by B*. This cost includes the exergy of the flow itself plus the irreversibilities that have been produced by all the processes made to produce that flow.

$$B^* = B + \sum I$$

Therefore, the cost of a flow increases when the processes that have been used to produce it are less efficient. Besides, it isn't a property that depends on the flow, it is a magnitude that depends also on the previous processes. Particularly, it depends on how the limits of the system are chosen. For instance, if the system of study is a thermic power plant, the cost of coal can be considered equal to its exergy, but if the system of analysis is extended to the mine, then cost is increased, since it is necessary to account for the exergy need for transportation and extraction too.

It is interesting to turn a exergetic cost into a dimensionless magnitude, dividing it by its exergy. This parameter is called unitary exergetic cost of a flow, and represents how many units of energy are required to produce an exergy unit of the flow:

$$k^* = \frac{B^*}{B}$$

Investigating what irreversibilities are the origin of the cost of a product goes beyond performing exergy balances, since it calls for a profound analysis: The process of costs formation. Its study constitutes an additional step to the conventional exergy analysis which is called exergetic cost accounting and represents the base of thermoeconomic analysis.

The relation between efficiency and cost becomes more visible when analyzing a simple process. If resources and products are measured in terms of exergy, the exergetic efficiency, η, is the inverse of the exergetic consumption of resources, κ, and this is, exactly, the exergetic cost of the product, k*.

$$\frac{1}{\eta} = \kappa = \frac{F}{P} = k^*$$

Nonetheless, it is not usual to study isolated processes, but connected among them. For example, figure C.1 shows a simple situation in which the product of process 1 is the fuel of process 2, which product is the fuel process 3 and so on.

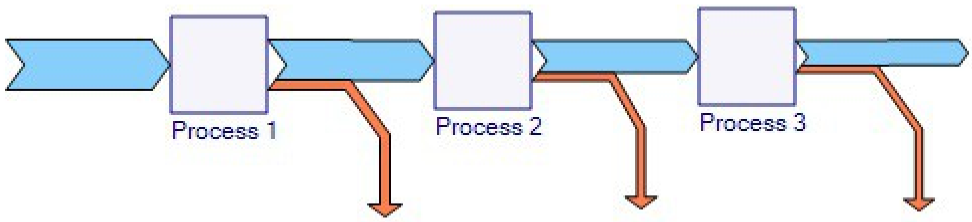

Figure C.1 Connected processes

To produce P_3, the product of the system, it's necessary to to consume F_3 local resources, so the unitary exergetic consumption of component 3 is $\kappa_3 = F_3/P_3$, but F_3 is the product of component 2, $F_3 = P_3$, and this goes on until F_1, which are the total resources that get into the system. Consequently the unitary exergetic cost of the system product is F_1/P_3.

$$k^*_{F,1} = 1$$

$$k^*_{P,1} = k^*_{F,1} = \kappa_1$$

$$k^*_{P,2} = k^*_{F,3} = \kappa_1 \kappa_2$$

$$k^*_{P,3} = \kappa_1 \kappa_2 \kappa_3$$

Always the unitary exergetic cost is higher than one, and it grows along with the complexity and/or inefficiency of the production structure of a given flow. In terms of exergetic cost we would have:

$$F^*_1 = F_1$$

$$P^*_1 = F_1 = P_1 + I_1$$

$$P^*_2 = F^*_2 = P_2 + I_1 + I_2$$

$$P^*_3 = F^*_3 = P_3 + I_1 + I_2 + I_3$$

As it can be seen in the equations above, the exergetic cost of a product is equal to its exergy plus the addition of of all the irreversibilities accumulated along the process.

To study the problem of cost calculation in complex situations which include several series and parallel processes along with recirculations, general methodologies are required. The first presented is the theory of exergetic cost, that provides rules that allow the construction of an equation system from which it is possible to obtain the cost of all the flows in a system. After that, the thermoeconomic analysis input-output is described, this analysis is based on a matrix formulation.

C.4. The theory of exergetic cost

According to economics, cost accounting has the function of gathering, measuring and organizing the information about how much things cost. In the case of exergetic cost accounting the predicament is similar, as it has to provide a rational method to assign the cost of products in terms of natural resources and their impact on the environment.

The main problem for exergetic cost assignation can be formulated as follows: given a system whose limits and aggregation level have been defined, included the diverse components that compose it. How to to obtain the costs of every flow that relate them?

The first step is defining the productive structure of our system. The physical structure of a system is the set of elements that are in it (for example, turbines, heat exchangers, boilers...) along with the material and energy flows between them. The productive structure, focuses on the purpose or function of the various components, allowing to introduce the concepts of purpose and efficiency about which we talked before. In this way, in a productive structure, every element consume some resources (F) coming from other components or the exterior, and originates a product (P) which is destined to other components or the exterior. Later examples will allow to see this in further detail.

Once the structure is defined, it is necessary to apply the rules of exergetic cost assignation discussed next.

When in a system, only one product is obtained, it is very simple to calculate its exergetic cost, as seen before. When the flow is intern, that is to say, it connects two components, the necessary exergy to produce it can be calculated as the sum of all the exergy consumptions in the previous components, until arriving to the incoming resources of the system. But several important questions come up: What happens when there are bifurcations? How are the costs distributed then?

Theory of exergetic cost supplies rules that allow to obtain the cost valued in term of exergy for flows in an energy system, independently of its complexity.

1) The exergetic cost of any flow depends on the costs of the incoming resources of the system. In the absence of exterior assignations, the cost of the incoming flows is its own exergy, or in other words, their unitary exergetic cost is one.

2) The cost of the product of each component of the system equals the sum of the exergetic cost of the flows that constitute the fuel of that component.

3) If the product of a component is made of several flows of the same exergetic quality, all of them have the same unitary exergetic cost, and therefor, we assign their exergetic cost proportionally to the exergy contained in them.

This set of rules to cost assignation are known as FP propositions and are equivalent to the cost properties described in input-output theory.

C.5. Input-output thermoeconomic analysis

Input-output thermoeconomic analysis, also called symbolic exergoeconomics is a methodology that combines exergetic cost theory and input-output analysis. Its objective is to obtain equations that relate the individual behavior of the processes that the components that constitute a system with its global behavior and annalize cost formation.

As seen previously, exergetic cost theory presents a method to determine the amount of resources necessary to obtain a product, using exergy as the criterion to distribute the cost. Input-output thermoeconomic analysis is based on the resolution of a system of equations expressed through matrix, making it very easy to implement in a matrix calculus software pack.

Since it is not necessary for this work, we will not get deep into the details of mathematical formulations. Only the most important concepts and equations will be discussed. It is important to remember that, originally, this type of analysis is a particular case of an input-output analysis, wich has been already studied, so the main changes regard formulation.

As said before, thermoeconomic analysis is based on the representation of the system that we want to study through its productive structure. In this structure, equipment, and physical flows are substituted by components and exergy flows between them that represent resources (fuel) and products. Generally, a component of the productive structure can encompass one or several components of the physical structure depending on the level of detail required for the study. For example, the purpose of a pump is to increase pressure in a fluid, so the product of that component will be the difference of exergies between the entrance and the exit of the component, and it will appear in the productive structure as one flow.

A productive structure is composed of *n* components, besides the environment which is considered component zero. The exergy flows that are part of f the product of component *i* and fuel *j* are represented as B_{ij}. We call P_i at the product of component *i*, and F_i the fuel of that component. Accordingly:

$$P_i = \sum_{j=0}^{n} B_{ij}$$

$$F_i = \sum_{j=0}^{n} B_{ji}$$

In the former equations, the summatory includes zero to take account of the exchange of flows with the environment. The *n*x1 vector that reflects the contribution of each of the n components to the final product is called P_s. The table that contains the value of all the B_{ij} elements, along with their sums by rows and columns is called fuel-product table.

Besides, the unitary exergetic consumption is defined as the number of exergy units required by each component, from the other components or the environment, to produce a unit of its product.

$$\kappa_{ij} = \frac{B_{ij}}{P_j}$$

The matrix (KP) is a *n*+1 square matrix whose elements are the unitary exergetic consumptions κ_{ij}. Unitary exergetic consumptions that make reference to the exterior κ_{0j} are placed in k_e vector.

Unitary exergetic cost of all the flows that are part of the product of each component have the same value (according to the rules of the theory of exergetic cost). The vector (*n*x1) where those unitary exergetic costs are shown is called k^*_p.

Through calculations similar to those of the input-output analysis two basic expressions are obtained. The first one allows to calculate all the products of the system from its final product:

$$P = \left(U - (KP)\right)^{-1} P_s$$

The second one gives back the unitary costs of the products of all the components:

$$k_p = \left(U - (KP)^T\right)^{-1} k_e$$

If the concepts and expressions above are analyzed carefully, it can be seen that they are completely analogous to those introduced by the input-output theory. There is an important difference though, which is that now exergy is used as measurement unit, introducing the second law of thermodynamics, that's why a different nomenclature is used.

Appendix D:

Exergy balances

There are many exergy balances along this work, and all of them share many characteristics. That is why in this section we will first expose the main flows that are taken into account for these balances, and how they are calculated. After that we will go through the calculated balances, showing the spreadsheets and discussing further their most relevant aspects.

D.1. Exergy Inputs

For the purposes of this work, we will consider an exergy input as any flow required by the agrarian sistem, or any other subsystem, to produce, that has an exergy value. This exergy value implies not only the exergy contained in the flow itself, but the one needed to make it available.

Among the flows that could be taken into account are the following: fuel, electricity, human labor, machinery, fertilizers, water, manure and animal traction. Though not all of them have finally been considered, given the small impact of some of them in industrialized agriculture or because of other factors.

The process of converting a flow into an exergy input is generally made by multiplying the amount of that flow in a given unit for its exergy content and an additional multiplier to take into account the exergy cost of availability.

To clarify this point we could imagine an example with a wood heater. If we wanted to know the exergy input of a traditional wood heater in the same way we are gonna do it for this work, we would have to consider the heat of combustion of the wood and multiply it for the amount of wood we use. But also it would be necessary to add the exergy needed to chop the wood, bring it back, or even the exergy cost of re-sharpening the axe if the wearing out was high enough. Considering that those costs are proportional to the recollected wood, we would multiply the exergy of the wood itsef by a given factor that can be normally obtained from bibliography.

$$\textit{Exergy Input} = \textit{Flow Amount} * \textit{Unitary Exergy} * \textit{Exergy Multiplier}$$

Given the magnitude of the flows that will be discussed, the exergy inputs will be generally expressed in tonnes of oil equivalent (toe) to allow a better understanding. A toe is the amount of energy released by burning one tonne of crude oil and its value according to the International Energy Agency is 41.868 GJ.

D.1.1. Fuel

The fuel needed to operate tractors and other harvesting equipment. The fuel used for this kind machinery is diesel fuel. As said before, its exergy is the sum of its own exergy and the one required by the extraction and industrial processing, transportation costs etc. To account for these extra costs a multiplier is applied to the heat of combustion to give the total exergy of diesel fuel. This multiplier is 1,134 and has been taken from Leach (Leach, 1978).

D.1.2. Electricity

The electricity consumption of the agrarian sector. Electricity has an obvious part in its exergy value, the amount of electric energy supplied to the consumer, but it has a high multiplier due to energy production and transportation. The multiplier has been taken as 3,6 (Naredo y Valero, 1999).

D.1.3. Human labor

The work made by human personal in farming activities. Since the agrarian sector in Spain is by now fully industrialized this flow can be neglect for the purposes of our calculations, as it is in every similar work studied.

D.1.4. Machinery

The embodied exergy of tractors and other farming machines. This exergy is obtained through the life cycle assessment of the average tractor (Classen, 2007). The value is taken as 135 MJ/kg for an average 3000 kg tractor of about 7000 hours of life duration. All tractors are considered average tractor for the purposes of calculation. This assumption is not exactly true but, as it will be seen later, the embodied exergy of machinery in the agrarian system is fairly small so we decided to settle for an approximation of this flow. To calculate the total annual exergy of this flow, the exergy contained in an average tractor is multiplied by the number of tractors bought that year.

D.1.5. Fertilizers

The exergy required to produce the fertilizers used in agriculture. The most commonly used fertilizers are nitrogen (N), phosphorus (P) and potassium (K). Out of the three only nitrogen is usually in pure state, with phosphorus and potassium being sold in compound forms: P_2O_5 and K_2O. Fertilizers used by the agriculture are generally a prepared mixture of those three, with a series of three numbers indicating the amounts of N, P_2O_5 and K_2O in which is called N-P-K rating.

Fertilizer production is a very energy-intensive process that carries with it an important amount of exergy, even if the exergy contained in the fertilizer itself is very small. The cumulative exergy required to produce a kilogram of nitrogen fertilizer and phosphorous fertilizer are obtained from Zornitza Kirova-Yordanova *(1998*)

D.1.6. Animal traction

The exergy required to breed and maintain working animals. Even more so that in the case of human labor, this flow can be overseen in the agrarian system of a fully industrialized society.

D.1.7. Manure

As manure disposal is one of the issues of current agriculture, this flow is considered a subproduct, that is to say it would be thrown away if not used as fertilizer, so the exergy necessary to produce it is zero. Additionally, for most of our exergy balances, we are considering systems in which the exergy flow that could be associated with manure would be an internal, recirculation flow, which wouldn´t get out of the system, neither as input nor as output of the system. That is why the manure exergy isn't considered in this work.

D.1.8. Water

Water requires exergy to be made available. Purifying, distribution, collection of water and other processes associated have an exergy cost. To account for all this exergy a value of 1,7 kWh/m3 is taken (Uche, Martinez y Carrasquer, 2011).

D.1.9. Fodder

The Spanish agrarian system is not self-sufficient. To feed the large quantities of cattle and other animal, huge amounts of fodder are required. Since the Spanish agriculture can provide for such high needs, fodder has to be imported. This turns imported fodder in an important input. In order to calculate its associated exergy we will assume that imported fodder is composed mainly of wheat and barley.

D.2. Exergy Outputs

Along this work, the considered outputs are always some form of edible product. The exergy, that is the useful energy of any food is its caloric value. Because of this, the exergy of the outputs can be calculated as the amount of the different products times their caloric value. The various caloric values of food are well known data that have been obtained from tables (USDA, 2013).

D.3. Exergy balances calculations

In this section, the spreadsheets of all the exergy balances that have not been shown in the main document will be presented. The calculations made to reach the exposed conclusions will also be described.

All of the production data are taken as the average value between years 2008 and 2009. This is done this way to decrease the inherent randomness of the agrarian system production, that can be altered by many parameters, such as annual precipitation or economic factors.

When not indicated otherwise, the different inputs and outputs of the systems will be calculated using the sources and methods described above in sections D.1 and D.2

D.3.1. Dry farming wheat

The spreadsheet and calculations for dry farming wheat have already been presented in the main document.

D.3.2. Irrigation wheat

Table D.1 shows the calculated flows for irrigation wheat. There is only one difference with the calculation of dry farming wheat, and that is, of course, the water input. The rest of the inputs have been obtained in the same way that in the case of dry farming wheat.

To calculate the exergy of the water input the first step was to obtain the water needs of irrigation wheat. The water need was taken from "Sistema de información agroclimática para el regadío" (SIAR, 2013). In the case of irrigation wheat in Spain for the years 2008 and 2009 the water needs are 477 mm (l/m2). Then the value of 1,7 kWh/m3 was applied as explained in section D.1 above.

Wheat 2008-2009	Irrigation		
	2008	2009	
Production [kt]	1.259	1.108	
Cultivated surface [kha]	278	243	
Total average electromechanical exergy [toe]			2.425.244
Electromechanical input [toe]			36.519
Water exergetic cost [kWh/m3]			1,7
Water annual needs wheat [mm]			477
Water annual total exergy cost [toe]			181.537
NPK 8-15-15 cumulative exergy [toe/t]			0,35
Urea 46 cumulative exergy [toe/t]			1,71
Fertilizer cumulative exergy [toe/ha]			0,67
Wheat fertilizer total exergy [toe]			174.300
Wheat exergy [Kcal/kg]			3.420
Total exergy input [toe]			392.355

Table D.1 Exergy balance of irrigation wheat

Knowing the exergy value of the water input, we can now calculate the exergy ratio as the output exergy divided by the sum of the three inputs. The exergy ratio of irrigation wheat is 1.1.

D.3.3. Rice

In the case of rice, the amount of fertilizer needed per hectare has been obtained from "fertilizer use by crop" (FAO, 2006) instead of "guia para la fertilización racional" (MAGRAMA, 2008). The FAO source had to be used since the Spanish document didn't have the fertilizer requirements of rice. This is probably dued to the small production of rice in Spain. The rest of the flows are calculated as before. The results can be seen bellow in table D.2.

Rice 2008-2009			
	2008	2009	
Production [kt]	634	914	
Cultivated surface [kha]	95	119	
Electromechanical input [toe]			15.035
Water annual needs wheat [mm]			748
Water annual total exergy cost [toe]			117.275
Fertilizer exergy [MJ/ha]			14.785
Fertilizer total exergy [toe]			37.872
Crop exergy [Kcal/kg]			3.600
Total exergy input [toe]			170.182

Table D.2 Exergy balance of rice

D.3.4. Corn

The process of calculation for the exergy balance of corn is identical to that of irrigation wheat, the sources and steps to follow are the same. Table D.3 allows us to see the results obtained for this balance.

Corn 2008-2009

	2008	2009	
Production [kt]	3.595	3.348	
Cultivated surface [kha]	349	325	
Electromechanical input [toe]			47.243
Water annual needs corn [mm]			596
Water annual total exergy cost [toe]			293.771
Fertilizer cumulative exergy [toe/ha]			0,61
Corn fertilizer total exergy [toe]			204.719
Corn exergy [Kcal/kg]			860
Total exergy input [toe]			545.733

Table D.3 Exergy balance of corn

D.3.5. Dry farming barley

The calculations for the exergy balance of dry farming barley are similar to those of dry farming wheat. The specific values and flows of this balance are presented in table D.4.

Barley 2008-2009	Dry farming		
	2008	2009	
Production [kt]	9.431	5.715	
Cultivated surface [kha]	3.072	2.658	
Electromechanical input [toe]			401.637
NPK 8-15-15 cumulative exergy [toe/t]			0,31
Urea 46 cumulative exergy [toe/t]			1,71
Fertilizer cumulative exergy [toe/ha]			0,33
Barley fertilizer total exergy [toe]			938.217
Barley exergy [kcal/kg]			3.540
Total exergy input [toe]			1.339.855

Table D.4 Exergy balance of dry farming barley

D.3.6. Cattle

The calculation method for cattle is different from that of cereals, It still follows the same principles explain in section D.1 though. Table D.5 shows the exergy value of the flows in the cattle subsystem.

Cattle 2008-2009		
	2008	2009
less than 12 months	2.028.000	2.095.000
12 to 24 months	759.000	707.000
More than 2 years	3.234.000	3.281.000
Dairy	808.000	828.000
Non-dairy	2.426.000	2.453.000
Dairy/beef cattle ratio		0,25
Nutrition needs for calves 200kg [Mj/d]		27
Nutrition needs for youngsters 350kg [Mj/d]		40
Nutrition needs for adults 450kg [Mj/d]		49
Total nutrition needs [toe]		1.055.581
Electric energy requirements dairy cattle [toe/cow]		0,27
Electric energy requirements beef cattle [toe/cow]		0,17
Water needs beef cattle [toe]		9.393
Water needs dairy cattle [toe]		1.964
Carcass total weight [t]		630.079
Milk production [hm3]		6,11
Exergy input dairy cattle [toe]		612.551
Exergy output dairy cattle [toe]		372.330

Table D.5 Exergy balance of cattle

The number and age state of all cattle has been obtained from “anuario de estadística” (MAGRAMA, 2011) and later the nutrition needs for each animal has to be assigned (UNICEN, 2013). Multiplying the nutritional needs and the number of each class of cattle we will get a caloric value. To obtain the exergy of that food it would be necessary to know the exact composition of the fodder given to animals. As this would be incredibly complex, given the large number of fodders, we make the assumption of considering the fodder made of wheat and barley, that are their main components in Spanish fodders (MAGRAMA 2003). Now we can apply the exergetic cost of wheat and barley, 0,5, as the multiplier to obtain the exergy flow.

Next we obtain the energy requirements of cattle (Irimia, Escudero y Alvarez, 2012) and apply the same multipliers for electricity that was seen in section D.1. Notice that the electric consumption of dairy cattle is higher, since it requires a device to milk it.

Water needs are obtained from “Agua para bebida de bovinos” (Sager, 2000) and its associated exergy is calculated as usual.

Carcass total weight and milk production (MAGRAMA, 2011) are the outputs of the system that are multiplied by their caloric value (USDA, 2013).

D.3.7. Poultry

In this section we study the exergy balance calculation of the chicken meat production subsystem. Table D.6 shows the main steps and magnitudes in the balance calculation.

Poultry 2008-2009	
Carcass total weight [t]	1.337.000
Feed to meet gain	1,91
Dressing percentage [%]	71
Liveweight[t]	1.883.099
Feed requirements [t]	3.596.718
Feed exergy input [toe]	622.152
Water requirements [m3]	6.474.093
Water exergy input [toe]	946
Electricity exergy input [toe]	113.801
Chicken meat caloric value [Kcal/kg]	2.150

Table D.6 Exergy balance of chicken meat production

Feed to meat gain, the amount of fodder in kg needed for the chicken to gain 1 kg of weight, and dressing percentage, the percentage of meat per kg o live chicken, are obtained considering broiler species (AVIAGEN, 2008)

With the carcass weight (MAGRAMA, 2011) and the dressing precentage we can calculate the liveweight, and subsequently the energy needs per ton of chicken from “Ahorro energético en granjas avícolas” (Oviedo-rondón, 2009)

D.3.8. Added agrarian system

The exergy balance of the agrarian system, taken in its aggregated form, is calculated next. Table D.7 allows to see the different intermediate values that lead to the obtaining of the exergy ratio.

Aggregated exergy balance 2008-2009		
Exergy inputs [ktoe]		
	Water	2.285
	Fertilizer	3.502
	Machinery	134
	Electrícity	1.368
	Fuel	923
	Fodder importation	1.864
	Total	10.077
Exergy outputs [toe]		
	Animal	2.051
	Vegetal	5.146
	Total	7.197

Table D.7 Exergy balance of the added agrarian system

In this case, all data has been obtained from "anuario de estadística" (MAGRAMA, 2011) except for the fodder importation (MAGRAMA, 2003). As for cattle, the exergy value of fodder has been calculated considering that it is composed mainly of wheat and barley.