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Evaluation of the Uncertainty in Thermoeconomic Input-Output Analysis Case Study: Anaerobic Digestion Plant

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Nomenclature

$\mathbf{A}$	Technical coefficients matrix
$\underline{\mathbf{A}}$	Difference between unit and technical coefficients matrixes
A	Annuity [€]
C	Cost [€] or [J]
$\dot{C}$	Cost rate on time basis [€/s] or [J/s]
CF	Cash flow [€]
CRF	Capital recovery factor
$\boldsymbol{E}$	Exergy based Input-Output matrix
$\mathbf{E}$	Exergy [J]
$\dot{\mathbf{E}}$	Exergy flow rate on time basis [J/s]
E	Energy [J]
$\dot{E}$	Energy flow rate on time bases [J/s]
F	Future value [€]
FCI	Fixed capital investment [€]
G	Gibbs function [J]
H	Operating time [h/y]
HHV	Higher heating value [MJ/kg]
$\mathbf{I}$	Identity or unit matrix
I	Cost index
IRE	Index of energy saving
$LCOE$	Levelized cost of electricity [€/kWh]
LHV	Lower heating value [MJ/kg]
Mm	Molar mass [$kg/kmol$]
N	Number of observations/iterations
P	Probability/Present value [€]
PEC	Purchased equipment cost [€]
Q	Heat [J]
$\dot{Q}$	Thermal power [W]
S	Entropy [J/K]
T	Temperature [K]
TCI	Total capital investment [€]
U	Internal energy [J]
V	Volume [m^3]
W	Work [J]
$\dot{W}$	Power [W]
X	General variable
$\boldsymbol{Z}$	Investment and O&M costs vector
$\dot{Z}$	Cost (investment, O&M) rate on time basis [€/s]
$\mathbf{b}$	Specific exogenous resources vector
$\mathbf{c}$	Specific cost vector
c	Specific cost rate on exergy basis [€/J] or [J/J]
$\mathbf{e}$	Specific exergy on mass basis [J/kg]

$\tilde{\mathbf{e}}$	Specific exergy on mole basis $[J/kmol]$
e	Specific energy on mass basis $[J/kg]$
f	Exergoeconomic factor
h	Specific enthalpy on mass basis $[J/kg]$
I	Interest/rate
$\dot{m}$	Mass flow rate on time basis $[kg/s]$
n	Mole $[kmol]$
$\dot{n}$	Mole flow rate on time basis $[kmol/s]$
p	Process vector
p	Pressure $[Pa]$
r	Relative cost difference
s	Specific entropy on mass basis $[J/kgK]$
t	Time [s]
u	Specific internal energy on mass basis $[m^3/kg]$/uncertainty
v	Exogenous resources vector
v	Specific volume on mass basis $[m^3/kg]$
$\bar{v}$	Speed $[m/s]$
w	Total inputs vector
x	Total outputs vector
x	Mole fraction $[kmol/kmol]$/generic quantity
y	Final demand vector
y	Mass fraction $[kg/kg]$
$\bar{z}$	Elevation $[m]$
Δ	Change, difference
δ	Perturbation
$\boldsymbol{\eta}$	Efficiencies vector
η	Efficiency
μ	Population mean
σ	Population standard deviation
τ	Retention time $[d]$
g	Gravitational acceleration module $[9.806\ m/s^2]$
R	Gas constant $[8314.5\ \frac{J}{kmol\ K}]$
$()_I$	First law of thermodynamics
$()_{II}$	Second law of thermodynamics
$()_0$	Dead state
$()_1$	Initial state
$()_2$	Final state
$()_b$	Boundaries
$()_C$	Cold
$()_c$	Combined system
$()_{\mathrm{cv}}$	Control volume
$()_{des}$	Destruction

$()_e$	Environment/exits
$()_{el}$	Electrical
$()_{env}$	Environmental
$()_{exc}$	Heat exchanger
$()_{exe}$	Exergetic
$()_F$	Fuel
$()_f$	Flow
$()_{gen}$	Generated
$()_H$	Hot
$()_i$	Inlets
$()_{in}$	In
$()_{los}$	Loss
$()_{\dot{m}}$	Accompanying mass flow rate
$()_N$	Normal conditions
$()_{out}$	Out
$()_P$	Product
$()_{\dot{Q}}$	Accompanying thermal power
$()_{ref}$	Reference
$()_{rev}$	Reversible
$()_{th}$	Thermal
$()_{tot}$	Total/overall system
$()_{\dot{W}}$	Accompanying power
$()^0$	Standard
$()^{ch}$	Chemical
$()^{CI}$	Capital investment
$()^{O\&M}$	Operating and maintenance
$()^{ph}$	Physical
$()^T$	Transpose matrix
$()^{SY}$	System
$\widetilde{()}$	Perturbed vector
$\overline{()}_{ln}$	Logarithmic mean

List of Acronyms

CHP	Combined Heat and Power
CRF	Capital Recovery Factor
CSTR	Continuous Stirred-Tank Reactor
FCI	Fixed Capital Investment
HHV	Higher heating value
IRE	Index of energy saving
IRR	Internal Rate of Return
JANAF	Joint Army and Navy Air Force
LCOE	Levelized Cost of Electricity
LHV	Lower heating value
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology
NPV	Net Present Value
O&M	Operating and Maintenance
PBP	Pay Back Period
PEC	Purchased Equipment Cost
TCI	Total Capital Investment
VIM	International Vocabulary of Metrology

Abstract

This thesis presents a method for the uncertainties evaluation and their propagation assessment in thermoeconomic Input-Output analysis since the problem of evaluating the uncertainty linked to thermoeconomic costs is highlighted by several studies. The context in question is that of the characterization and the description of the natural, exergy resources necessary in production chains to yield commodities. The key concepts of exergy and economic cost are used together into thermoeconomics to analyse the costs of each product and to optimize individual components or entire systems. Thermoeconomic analysis may be accompanied and strengthened by the uncertainty analysis thanks to the use of statistical techniques as the Monte Carlo simulations. The latter allows to quickly estimate the intervals of values in which the results of the thermoeconomic Input-Output analysis will fall whenever the input data needed to perform the analysis suffer from some uncertainty. The studied methodology is then applied to an existing anaerobic digestion plant to provide an application example. The thermoeconomic analysis is carried out successfully in order to run a design evaluation of the plant and an uncertainty evaluation of resulted values.

Key words: *uncertainty*, *thermoeconomics*, *Input-Output*, *cost*, *design evaluation*, *optimization*, *sustainability*.

Sommario

Dacché il problema della valutazione dell'incertezza legata ai costi termoeconomici è evidenziata da diversi studi, questo lavoro si propone di presentare un metodo per la valutazione delle incertezze e della loro propagazione nell'analisi termoeconomica con approccio Input-Output. Il contesto considerato è quello della caratterizzazione delle risorse naturali, energetiche necessarie nei processi produttivi di beni. I concetti principali dell'exergia e del costo economico sono impiegati nella termoeconomia al fine di analizzare i costi di ogni prodotto e per ottimizzare singoli componenti o interi sistemi produttivi. L'analisi termoeconomica può essere accompagnata e rafforzata dall'analisi dell'incertezza grazie all'utilizzo di tecniche statistiche come le simulazioni Monte Carlo. Esse permettono di stimare rapidamente gli intervalli di valori in cui i risultati dell'analisi termoeconomica con approccio Input-Output cadranno ogniqualvolta i dati necessari per eseguire l'analisi siano affetti da una qualche incertezza. La metodologia studiata è poi applicata a un impianto reale di digestione anaerobica come esempio applicativo. L'analisi termoeconomica viene eseguita con successo al fine di fornire un'analisi di design dell'impianto e una valutazione dell'incertezza dei valori dei risultati.

Parole chiave: *incertezza*, *termoeconomia*, *Input-Output*, *costo*, *analisi di design*, *ottimizzazione*, *sostenibilità*.

Introduction and scope of work

Engineering proposes models to study and solve significant problems for the society. All the instruments needed to gather, analyze and interpret information and data must be used considering that these are characterized by *variability* [1] as the successive observations of a system or of a phenomenon does not produce exactly the same result, the data collected may not be known with certainty, different assumptions may lead to different results. So, being able to recognize and to describe the uncertainty of a quantity is important to strengthen a model and to be able to use it more properly.

In the last decades there has been an increasing awareness on the fact that the financial costs of materials and products do not provide a condign description of the resources needed for their production [2]. The economic analysis considers the *scarcity* of goods in the market but does not consider sufficiently the consumption of resources required to produce them. To take account of *sustainability* of a production process, economic analysis has to be accompanied with another investigation that considers a non-monetary dimension [3].

Thermoeconomics is that branch of engineering that combines exergy analysis and the economic principles in order to calculate the costs of each product of a production chain and to optimize individual components or entire systems [4]. These costs may be:

- *Exergetic costs [J/J]*, whenever exergy is both the physical quantity of the product in question and the quantity which quantifies the expenditure of resources necessary to produce it;
- *Exergoeconomic costs [€/J]*, whenever exergy is the quantity characterizing the product but the expenditure on needed resources is evaluated as monetary outlay.

The problem of evaluating the uncertainty linked to thermoeconomic costs is highlighted by several studies; from literature [5] and engineering practice [6] the importance of knowing how to apply useful methodologies for *uncertainty evaluation and propagation* is glaring.

The aim of this study is to provide a method for the assessment of the uncertainty in estimating the thermoeconomic costs. This method is based on statistical techniques that work knowing the probability distribution of the uncertainty. *Monte Carlo simulations* can be used to quickly analyze a large number of cases [7] in which variability affects data or different choices and assumptions are made. Verification of results of thermoeconomic analysis, when some assumptions have been changed, leads to the border of the sensitivity analysis [6].

Thesis structure is composed by five parts:

1. *Chapter 1*. The concept of exergy is introduced since it can be used as an instrument to assess the quality of an energetic process and its ability to destroy energy;
2. *Chapter 2*. Thermoeconomics is presented with an Input-Output approach (representing the state of art) in which the thermoeconomic system can be studied and solved with a matrixes arrangement borrowed from economics;
3. *Chapter 3*. After a brief treatise on uncertainty key concepts, sources and propagation, a method for uncertainty evaluation in thermoeconomic Input-Output analysis is provided;
4. *Chapter 4*. Case study is introduced as an application example of the uncertainty evaluation method. This concerns the analysis of an existing anaerobic digester for the production of biogas from a mixture of maize silage and pig slurry. The plant is equipped with an engine for the cogeneration of electrical and thermal power. Then, the thermodynamic and economic models of the plant have been built and the uncertainties in the study of the digester have been gathered and described;
5. *Chapter 5*. Thermoeconomic input-output analysis is carried out with uncertainty assessment on exergoeconomic cost analysis for the case study as well as uncertainty study on the assumptions of the model. A design evaluation is performed.

Even through the application to the case study, it is possible to understand that thermoeconomic analysis is of central importance for the characterization of the material and economic resources needed to yield products in any system. However, such an analysis must be accompanied by a consistent uncertainty appraisal to assess the variability linked to results and to perform a critical evaluation. In fact, some assumptions may affect the validity of the results and this is as truer as the system inefficiencies are larger. Moreover, it has come to light, once the uncertainty is characterized, how such a method for Input-Output analysis represents a general formalization applicable to any system; for example to supply chain analysis.

1. Exergy Concepts and Analysis

The *conservation of mass* and *conservation of energy* principles are used, together with the *second law of thermodynamics*, in exergy analysis for the design and analysis of thermal and energetic systems [8] in order to understand how to use efficiently natural resources. Unlike energy, exergy is *not conserved*: it can be transferred to or from a system and irreversibilities can also destroy it. So exergy analysis can be used to *individuate inefficiencies* and to realize an improved resources utilization. After presenting the fundamentals of physical exergy, the exergy concept is extended considering the role of chemical composition. At last it is presented some mention of the use of exergy for the analysis of systems.

1.1. Exergy notion

Whenever two systems are brought into communication there is the possibility of extracting work as they are allowed to come into equilibrium. If one of the two systems is the environment, an idealized reference environment, and the other one is some system of interest, then exergy is the *maximum theoretical work* obtainable while they interact to equilibrium and its numerical value depends on the state and the condition of the system of interest and the environment [9]. Everything not included in the system, in the portion of the surroundings where the intensive properties do not vary during any process involving the system and its closer surroundings, is considered *environment*.

Not to complicate too much the model used to approximate the reality of the processes which can be described in a exergy analysis, it is often sufficient to represent the environment as a simple compressible part of the physical world, large in extent, uniform in temperature T_0 corresponding to 298.15 K, and in pressure p_0, corresponding to 101325 Pa, and free of irreversibilities. When a closed system, which always contains the same matter, is in equilibrium with the environment, the state of the system is defined as *dead state*. At this state, even if both the system and the environment possess energy, the value of exergy is zero because the system and its surroundings cannot interact with each other and it is not possible a spontaneous change within both of them.

1.1.1. Exergy of a system

The expression used to evaluate exergy can be derived by studying the system given in Figure 1.1 for which it is possible to imagine a process in which the closed system reaches the dead state.

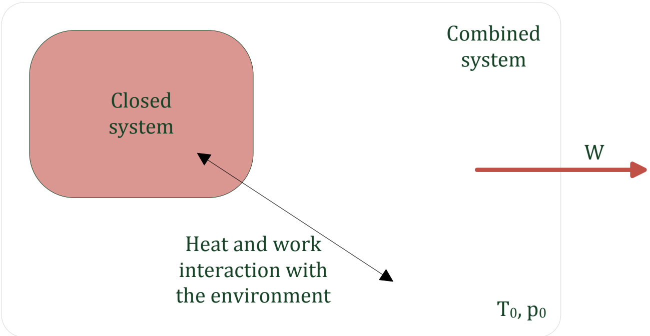


Figure 1.1 – Closed system and environment as a combined system

By considering only a work exchange, the energy balance for the combined system becomes

$$\Delta E_c = W_c \tag{1.1}$$

in which the energy change of the combined system equals the developed work exchanged between the closed system and the environment. The kinetic and potential energy are evaluated relatively to the environment, thus the energy of the closed system at the dead state is just corresponding to its internal energy. Therefore the energy change can be expressed as

$$\Delta E_c = \left(U_0 - E\right) + \Delta U_e \tag{1.2}$$

where the last term represents the internal energy variation for the environment. To express this term, it is possible to use one of the $T\ dS$ equations that allow to determine entropy changes from other property data which can be more easily defined. Considering a pure, simple compressible system undergoing an internally reversible process, $T\ dS$ represents the heat transfer at a part of the system boundary. This heat, without an overall system motion and the effect of gravity, from an energy balance is equal to the differential of the internal energy plus the work of an internally reversible process. The latter, by definition of simple compressible system is given by the expression $p\ dV$, so the first $T\ dS$ equation results

$$T\,dS = dU + p\,dV$$

and for the environment, in which extensive properties can change because of the interactions with other systems, since T_0 and p_0 are constant, it takes the form

$$\Delta U_e = T_0\,\Delta S_e - p_0\,\Delta V_e$$

Using this equality to replace ΔU_e into Equation (1.2), it results

$$\Delta E_c = \left(U_0 - E\right) + \left(T_0\,\Delta S_e - p_0\,\Delta V_e\right) \tag{1.3}$$

Consequently, the work developed by the combined system, merging Equations (1.1) and (1.3), gives

$$W_c = \left(E - U_0\right) - \left(T_0\,\Delta S_e - p_0\,\Delta V_e\right)$$

Since the total volume of the combined system is constant, the change in volume of the environment is opposite in sign but equal in magnitude to the volume change of the closed system, so

$$W_c = \left(E - U_0\right) + p_0\left(V - V_0\right) - T_0\,\Delta S_e \tag{1.4}$$

The maximum theoretical work is then determined using the entropy balance that, for the combined system, reduces to give only

$$\Delta S_c = S_{gen}$$

because there is not heat transfer at the boundary of the combined system. The term S_{gen} is linked with the generation of entropy due to irreversibilities as the closed system comes into equilibrium with the environment. The entropy change can also be written as the sum of the difference between the entropies of the closed system at the dead state and at the given state and the entropy change of the environment

$$S_{gen} = \left(S_0 - S\right) + \Delta S_e \tag{1.5}$$

Substituting Equation (1.5), solved for ΔS_e, into Equation (1.4) it gives

$$W_c = \left(E - U_0\right) + p_0\left(V - V_0\right) - T_0\left(S - S_0\right) - T_0\, S_{gen}$$

Accordingly the *exergy of a system*, **E**, as the maximum theoretical value for the work of the combined system at a specific state is given by the expression

$$\mathbf{E} = \left(E - U_0\right) + p_0\left(V - V_0\right) - T_0\left(S - S_0\right) \tag{1.6}$$

in which E represents the energy, sum of the internal, kinetic end potential energies, V the volume and S the entropy of the system besides U_0, V_0 and S_0 denotes the same properties at the dead state and the term $T_0\ S_{gen}$ is set to zero. Exergy is *independent of the details of the process* linking the given and the dead states of the system and depends only on this two end states of the closed system. The term $T_0\ S_{gen}$, instead, depends on the nature of the process of the closed system to the dead state and is positive in the presence of irreversibilities.

Exergy is an *extensive property* of the system and its value, which has the *unit of measurement of work*, can be evaluated once the environment is specified. Exergy cannot be negative, a system is able to change spontaneously toward the dead state and no work must be done to effect such a change. In a spontaneous process without the will to obtain work, exergy is completely destroyed when the system reaches the dead state. The *specific exergy on a unit mass basis*, **e**, is, from Equation (1.6), given by

$$\mathbf{e} = \left(e - u_0\right) + p_0\left(v - v_0\right) - T_0\left(s - s_0\right) \tag{1.7}$$

where all properties are specific on mass basis; considering the kinetic and potential energies as parts of the energy at the given state, Equation 1.7 can be rewritten as

$$\mathbf{e} = \left(u - u_0\right) + p_0\left(v - v_0\right) - T_0\left(s - s_0\right) + \frac{\overline{V}^2}{2} + g\overline{z} \tag{1.8}$$

so the units of the specific exergy are the same as those of the specific energy. Moreover, the *exergy change between two state* of a closed system can be written, using Equation (1.6), as the difference

$$\mathbf{E}_2 - \mathbf{E}_1 = \left(E_2 - E_1\right) + p_0\left(V_2 - V_1\right) - T_0\left(S_2 - S_1\right) \tag{1.9}$$

When the value of exergy is zero a system is at the dead state and therefore it is in thermal and mechanical equilibrium with the environment: the thermomechanical contribution to exergy is zero but the matter of the system can enter into chemical interaction with some environmental components developing additional work. The distinction between physical and chemical exergy is then discussed.

1.1.2. Exergy balance

The *closed system exergy balance* may help to study the irreversibilities and exergy changes providing the basis for exergy analysis. Such a balance is developed by combining the closed system energy and entropy balances in the forms expressed by Equation 1.9 in which heat and work are transferred to system surroundings, not necessarily involving the environment, and for which entropy balance is multiplied by the temperature T_0 and subtracted from the energy balance:

$$\left(E_2 - E_1\right) - T_0\left(S_2 - S_1\right) = \int_1^2 \delta Q - T_0 \int_1^2 \left(\frac{\delta Q}{T}\right)_b - W - T_0 S_{gen} \tag{1.10}$$

where T_b represents the temperature at the system boundaries on which δQ is received and the term S_{gen} is due to internal irreversibilities. The closed system exergy balance results rearranging Equation (1.9), collecting the terms involving δQ and using Equation (1.8), so

$$\left(\mathbf{E}_2 - \mathbf{E}_1\right) - p_0\left(V_2 - V_1\right) = \int_1^2 \left(1 - \frac{T_0}{T_b}\right) \delta Q - W - T_0 S_{gen}$$

$$\mathbf{E}_2 - \mathbf{E}_1 = \left\{ \int_1^2 \left(1 - \frac{T_0}{T_b}\right) \delta Q - \left[W - p_0\left(V_2 - V_1\right)\right] \right\} - T_0 S_{gen}$$

exergy change is given by the difference between exergy transfers, the term between the braces, and the exergy destruction. This balance can be used instead of the entropy balance as an expression of the second law. Exergy transfers is represented by two terms, the first one, the integral, is linked with heat transfer to or from the system during the process while the term in square brackets can be seen as the exergy transfer accompanying work.

By the second law, *exergy destruction* of a process is positive when irreversibilities are present within the system or, at the minimum, can vanish in the limiting case with no irreversibilities. Thus exergy destruction, that is not a property, cannot be negative, instead, exergy change is a property of a system and consequently it can assume any sign. Exergy balance can play an important role in developing new strategies for more effective fuel use as it can be used to determine positions, kinds and magnitudes of energy resource waste.

For particular analysis a convenient form of the exergy balance is the *closed system exergy rate balance*

$$\frac{d\mathbf{E}}{dt} = \sum_j \left(1 - \frac{T_0}{T_j}\right)\dot{Q}_j - \left(\dot{W} - p_0 \frac{dV}{dt}\right) - T_0 \dot{S}_{gen} \tag{1.11}$$

where the term at the first member is the time rate of exergy change; the first term at the second member represents the time rate of exergy transfer accompanying heat transfer at the rate $\dot{Q}_j$ on the boundary; the second term consists of the time rate of energy transfer by work and of the contribution linked to the time rate of change of system volume; the last term at the second member accounts for the time rate of exergy destruction and is subsequently related with entropy generation.

1.1.3. Flow exergy

The concept of flow exergy is central in the introduction of the exergy rate balance for a control volume, the mathematical abstraction representing the system in question. An exergy transfer accompanies flow work and mass flow every time the latter across the boundary of a control volume. Introducing enthalpy in Equation (1.8), *specific flow exergy* is, indeed, given by

$$\mathbf{e}_f = (h - h_0) - T_0(s - s_0) + \frac{\bar{V}^2}{2} + g\bar{z}$$

where h and s represent respectively specific enthalpy and entropy at the inlet or exit considered and h_0 and s_0 represent the values of this properties at the dead state.

When mass flows across the boundary of a control volume, there is an associated energy transfer given by

$$\dot{E}_{\dot{m}} = \dot{m}\, e = \dot{m}\left(u + \frac{\overline{V}^2}{2} + g\overline{z} \right)$$

with e as the specific energy evaluated at the inlet or exit under consideration. Similarly it is possible to consider the time rate of exergy transfer accompanying mass flow

$$\dot{\mathbf{E}}_{\dot{m}} = \dot{m}\,\mathbf{e} = \dot{m}\left[\left(e - u_0\right) + p_0\left(v - v_0\right) - T_0\left(s - s_0\right) \right]$$

One-dimensional flow is assumed. At location where mass enters or exits a control volume, in addition to an exergy transfer accompanying mass flow, an exergy transfer accompanying flow work takes place according to

$$\dot{\mathbf{E}}_{\dot{W}} = \dot{m}(pv - p_0 v)$$

Flow work is given, on a time rate base, by the product of mass flow rate multiplied by the specific volume at the inlet or exit and by the pressure. As transfers of exergy accompanying mass flow and flow work occur at locations where mass enters or exits a control volume, a *single expression which considers both the effects* is convenient and given by

$$\dot{\mathbf{E}} = \dot{m}\,\mathbf{e}_f = \dot{m}\left[\left(e - u_0\right) + p_0\left(v - v_0\right) - T_0\left(s - s_0\right) + \left(pv - p_0 v\right) \right]$$

The term $\mathbf{e}_f$ represents the specific flow exergy rewritten underlining, per unit of mass, the exergy transfer accompanying mass flow and flow work, making explicit energy as the sum of internal, kinetic and potential energy it is finally possible to reconnect to the original form expressed at the beginning of the subparagraph. Flow exergy evolves in a similar way as does enthalpy in the development of the control volume energy rate balance, each quantity is a sum consisting of a term associated with the flowing mass and a contribution linked to flow work at the inlet or exit under consideration.

1.1.4. Exergy rate balance

For engineering analysis, it is important to extend the concept of exergy balance, with the introduction of flow exergy, to a control volume, transforming the closed system form. Modifying Equation (1.11), to account for the exergy transfers just described at inlets and exits, it is possible to write the *control volume exergy rate balance*

$$\frac{d\mathbf{E}_{cv}}{dt} = \left[\sum_j \left(1 - \frac{T_0}{T_j}\right)\dot{Q}_j - \left(\dot{W}_{cv} - p_0 \frac{dV_{cv}}{dt}\right) + \sum_i \dot{m}_i \mathbf{e}_{f,i} - \sum_e \dot{m}_e \mathbf{e}_{f,e} \right] - T_0 \dot{S}_{gen}$$

where the subscripts i and e denote inlets and exits respectively. The term at first member represents the time rate of change of the exergy of the control volume, the term in square brackets represents the rate of exergy transfer and the last term at second member the rate of exergy destruction due to irreversibilities within the control volume. In particular, the term in square brackets is composed by exergy transfer rate accompanying heat transfer at the location on boundary where the instantaneous temperature is T_j; exergy transfer rate accompanying work other than flow work and due to volume change; exergy transfer accompanying mass flow and flow work at the inlets and at the exits with the assumption of one-dimensional flow at the openings on boundaries.

At steady state exergy and volume changes over time are equal to zero so the equation indicates that the rate at which exergy is transferred into the control volume must exceed the rate at which exergy is transferred out, the difference is therefore the rate at which exergy is destroyed within the control volume due to irreversibilities. Hence, at steady state, the rate of exergy transfer accompanying the power $\dot{W}_{c\,v}$ is the power itself.

1.1.5. Chemical exergy

Considering the role of chemical composition of elements that enters or exits from the control volume considered, it is possible introduce another aspect of exergy: for example seeing in the system a specified amount of a fuel at temperature T_0 e pressure p_0 and air in the environment. Since the system is in thermal and mechanical equilibrium with the environment, the value of physical exergy is, as defined, zero. More precisely, the thermomechanical contribution to the exergy magnitude has a value of zero, but the chemical contribution related to composition has a value other than zero.

Referring to the example, the problem is to evaluate the work obtainable by allowing the fuel to react with the oxygen from the air to produce the environmental components carbon dioxide and water, each at its respective state in the environment. *Chemical exergy* is, thus by definition, the maximum theoretical work that could be developed by the combined system. The sum of the thermomechanical or physical and chemical exergy is the total exergy associated with a given system at a specific state of interest, relative to a specific exergy reference environment.

To evaluate the chemical exergy of a generic substance it is imaginable to consider a fuel cell in which the material, at the dead state, and air interact. Assuming the environment consists of an ideal gas mixture, the oxygen enter at its condition within the air: temperature T_0 and partial pressure given by the product of p_0 multiplied by the mole fraction of the oxygen in the exergy reference environment. This way, chemical exergy is the maximum theoretical work that could be developed by a fuel cell into which a substance of interest enters at the dead state and reacts completely with environmental components to produce environmental components. For an ideal gas mixture at the dead state consisting only of substances present as gases in the environment, the chemical exergy is obtained by summing the contributions of each component. The result, per mole of mixture, is

$$\tilde{e}^{ch} = \tilde{R}\,T_0 \sum_j x_j \ln\left(\frac{x_j}{x_{e,j}}\right)$$

where $\tilde{R}$ is the molar gas constant, x_j and $x_{e,j}$ represents the mole fraction of a j^{th} component in the mixture at the dead state and in the environment respectively. Rewriting the logarithmic term using logarithms rules, *chemical exergy for ideal gas mixtures* can be expressed as

$$\tilde{e}^{ch} = \sum_j x_j \tilde{e}_j^{ch} + \tilde{R}\,T_0 \sum_j x_j \ln x_j$$

For many cases of interest the environment typically considered must be extended to include other substances. Once the environment is determined, a series of calculation would be required to obtain exergy values for the substances of interest; these complexities can be overcome by using a table of standard chemical exergies. *Standard chemical exergy* values are based on a standard exergy reference environment at T_0 298,15 K and pressure p_0 101325 Pa. The reference environment also consists of a set of reference substances with standard concentrations reflecting as closely as possible the chemical makeup of the natural environment. To exclude the possibility of developing work from interactions among parts of the environment, the reference substances must be in equilibrium mutually. They are usually divided into three groups: gaseous components of the atmosphere, solid substances from the Earth's crust and ionic and non-ionic substances from the oceans.

The methods employed to determine the tabulated standard chemical exergy values vary depending on the specific table but since there is no one specification of the environment that suffices for all applications, one must be careful to the word 'standard' even if there is generally a good agreement. The convenience of using standard values generally outweighs the slight lack of accuracy that might result; in particular, the effect of slight variations in the values of the reference dead state about their standard values can be neglected.

The standard chemical exergy of a substance not present in the environment can be evaluated by considering an idealized reaction of the substance involving other substances for which the chemical exergies are known. It is possible, in principle, to determine this standard chemical exergy, considering a reaction of the substance involving other substances for which the standard chemical exergies are known, it writes

$$\tilde{\mathbf{e}}^{0ch} = -\Delta G + \sum_{P} n\,\tilde{\mathbf{e}}^{0ch} - \sum_{R} n\,\tilde{\mathbf{e}}^{0ch}$$

with the negative of the change in Gibbs function, $-\Delta G$, for the reaction of the substance in question with the matter of the environment, and the other terms evaluated using the known standard chemical exergies, considering the moles of these reactants (subscript R) and products (subscript P).

1.1.6. Total exergy

The exergy associated with a specific state of a system is hence the sum of two contributions: the physical and the chemical exergy. On a unit mass basis the *total exergy* is

$$\mathbf{e} = \left(u - u_0\right) + p_0\left(v - v_0\right) - T_0\left(s - s_0\right) + \frac{\overline{V}^2}{2} + g\overline{z} + \mathbf{e}^{ch}$$

Likewise the specific flow exergy associated with a specific state is the sum

$$\mathbf{e}_f = \left(h - h_0\right) - T_0\left(s - s_0\right) + \frac{\overline{V}^2}{2} + g\overline{z} + \mathbf{e}^{ch}$$

When evaluating the thermomechanical contribution it is like thinking of treating the system without change in composition from the specified dead state, in the condition where it is in thermal and mechanical equilibrium with environment; depending on the nature of the system, this may be a hypothetical condition.

1.2. Exergy analysis

Devices designed to do work by utilization of a combustion process, such as vapour and gas power plant and internal combustion engines, always have irreversibilities and losses associated with their operation. *Exergy analysis* is useful for assessing the fact that actual devices produce work equal to only a fraction of the maximum theoretical value that might be obtained in idealized circumstances. Several discussions [10] have been conducted about sustainable development, greenhouse gas emissions, environmental impact and renewability of energy resources, however, the concept of renewability has been often associated to mass and energy balances, not taking into account the reduction of the quality of the energy, or exergy destruction, related to energy conversion processes.

The traditional definition of *sustainability*, that calls for policies and strategies that satisfy society present needs without compromising the ability of future generations to satisfy their own needs, does not provide a rational way to quantify this ability. As Szargut [11] and Wall [12] stated, exergy, which originates from the contrast between sun and space, drives flows of energy and matter on the surface of the Earth. This exergy input is destroyed in order to keep the natural cycles responsible for recycling materials on the surface, and a small part is stored as fossil fuels and mineral ores. Recycling takes time and exergy to be accomplished, but total recycling is not possible due to the second law of thermodynamics. Currently, since human development is based on the consumption of fossil fuels at a greater rate than that at which the deposit of fossil fuels have been generated and since total recycling is not possible, it is imperative to seek for technologies that make better with less use of exergy available from all sources.

1.2.1. Exergetic efficiency

Exergetic efficiency expressions can take many different forms. Anyhow its value can be derived by the use of the exergy rate balance, assuming a control volume at steady state and considering the thermal power transfer through the use of the *Carnot factor* to be able to compare it directly with the exergy transferred due to work or mass flow.

$$\dot{\mathbf{E}}_{\dot{Q}} = \left(1 - \frac{T_0}{T_j}\right)\dot{Q}_j$$

Commonly [13] it is possible to indicate a general expression for the *second law efficiency* that is

$$\eta_{II} = \frac{W}{W_{rev}}$$

where at the numerator is considered the useful effect of the system analysed generally produced within the control volume for the outside and therefore according to classical thermodynamics, work; at the denominator, instead, is considered the reversible work i.e. that work ideally available considering a reversible process without irreversibilities, with an entropy change of the system that depends only on heat exchanges on the control volume. Therefore the denominator represents the maximum useful effect which can be obtained with ideal machines and processes within the meaning of the second law.

Exergetic efficiency can be used to evaluate the effectiveness of engineering measures taken to improve the performance of a thermal system. It also can be used to measure the potential for improvement in the *performance* of a given thermal system by comparing the efficiency of the system to the efficiency of alike systems; important differences between these values would suggest that improved performance is possible. The limit of 100% exergetic efficiency should not be regarded as a practical objective. To achieve such an idealized processes might require extremely long times to execute process and/or complex devices, both of which are at odds with the objective of profitable operation. Decisions usually take into accounts total costs, indeed, an increase in efficiency to reduce fuel consumption or utilize resources better, requires additional expenditures normally for facilities and operations. The choice between fuel savings and additional investment habitually leads to a lower efficiency which could be spared using the best available technology. To improve energy resource utilization there are various methods that try to achieve their aims cost-effectively:

- *cogeneration*, sequentially produces electrical and thermal power for the desired use through a system as integrated as possible, with a total expenditure that is less than would be required to develop them separately;
- *power recovery*, can be realized by inserting a turbine into a pressurized gas or liquid stream to capture some of the energy that would otherwise be destroyed in a spontaneous expansion;
- *waste heat recovery*, contributes to overall efficiency by using some of the exergy that would otherwise be discarded to the surroundings, as for the exhaust gases of internal combustion engines.

1.2.2. Introducing thermoeconomics

Principles of *thermodynamics* together with fluid mechanics, heat transfer, materials, manufacturing applications and engineering *economics* are the bases for the design of thermal systems.

A simple example that illustrates the use of the exergy and cost concepts in design is that of considering a heat exchanger. From the second law of thermodynamics it is imaginable to see the average temperature difference between the two streams passing through the exchanger as a measure of irreversibilities because they would vanish as the temperature difference approached zero. For the system, the source of exergy destruction exacts an economic penalty in terms of fuel cost, so the cost increases with increasing the temperature difference. To reduce irreversibilities it is possible to extend heat transfer area, but more area means a larger, more costly heat exchanger i.e. a greater capital cost. Hence this cost decreases as temperature difference increases. The total cost is the sum of the capital cost and the fuel cost; the minimum cost will be, so, a compromise between the will to minimize capital and fuel costs that have contrasting trends.

The actual *design process* can differ significantly from this simple case [9]: it can happen that costs cannot be determined precisely or fuel price may vary widely over time, and equipment cost can be difficult to predict. Generally equipment cost would not vary continuously, moreover thermal systems consist of several components that interact with one another, and usually optimization of components individually does not guarantee an optimum for the overall system. Moreover, several design variables must often be considered and optimized simultaneously.

2. Thermoeconomic Input-Output Analysis

Thermoeconomics is the branch of engineering that combines *exergy analysis* and *economic principles* to provide the designer or operator of the system with information and crucial details not available through conventional analyses but important to the design and operation of a cost-effective system [4]. Since the concept of exergy is fundamental for this kind of analysis, the term exergoeconomics can also be used to describe the combination of exergetic assessment and economics that can be seen as a exergy-aided cost minimization. The objectives of a *thermoeconomic analysis* are:

- to estimate separately the costs of each product generated by a system that have more than one product;
- to understand the cost formation process and the flow of costs in the system;
- to optimize specific variables in a single component;
- to optimize the overall system.

After a discussion on the basic elements of thermoeconomics; cost balances as well as the use of exergoeconomic variables are presented, for the evaluation and optimization of the design of thermal systems. Then the Input-Output methodology is applied to the thermoeconomics analysis through the introduction of the matrixes arrangement to estimate the exergetic and exergoeconomic cost of products.

2.1. Fundamentals and exergy costing

Enterprise cost accounting mainly concerns with the determination of the actual cost of products or services, the supply of a rational basis for pricing goods or services, a means for allocating and controlling expenditures as well as information on which operating decisions can be evaluated and based. From here comes the use of cost balances: in a conventional economic analysis, for an overall system operating at steady state, a *cost balance* is formulated this way

$$\dot{C}_{P,tot} = \dot{C}_{F,tot} + \dot{Z}_{tot}^{CI} + \dot{Z}_{tot}^{O\&M} \tag{2.1}$$

with the subscript *tot* referred at the overall system. Cost balance expresses the cost rate of the product of the system as the total rate of expenditures made to generate the product itself, so the fuel cost rate, the cost rate associated with capital investment and the cost rate associated with operating and maintenance (O&M). The rates associated to capital investment and O&M are calculated by dividing the annual contribution of capital investment and the annual O&M costs, individually, by the number of time units, usually hours, of system operation per year; the sum of these two variables is denoted by

$$\dot{Z} = \dot{Z}_{tot}^{CI} + \dot{Z}_{tot}^{O\&M} \tag{2.2}$$

At steady state, a system can have a number of entering and exiting material stream as well as both heat and work interaction with the surroundings. To these transfers of matter and energy are associated exergy transfers into and out of the system and exergy destructions caused by the irreversibilities within the system. Costs should only be assigned to commodities of value while exergy, gauging the effects of irreversibilities, is meaningfully used as a basis for assigning costs in thermal systems. In fact, thermoeconomics rests on the notion that exergy is the only rational basis for assigning costs to the interactions that a thermal system experiences with its surroundings and to the sources of inefficiencies within it. This approach is called *exergy costing*.

This way a cost is associated with each exergy stream. Hence, for the entering and exiting streams of matter with associated rates of exergy transfer, for the power and for the exergy transfer rate associated with heat transfer, it is possible to write respectively

$$\dot{C}_i = c_i \, \dot{\mathbf{E}}_i = c_i \left(\dot{m}_i \, \mathbf{e}_i \right)$$

$$\dot{C}_e = c_e \, \dot{\mathbf{E}}_e = c_e \left(\dot{m}_e \, \mathbf{e}_e \right)$$

$$\dot{C}_{\dot{W}} = c_{\dot{W}} \, \dot{W}$$

$$\dot{C}_{\dot{Q}} = c_{\dot{Q}} \, \dot{\mathbf{E}}_{\dot{Q}}$$

where the subscripts *i* and *e* denotes inlets and exits but, above all the *c* represents *average costs per unit of exergy* in euro per Joule.

Exergy costing involves cost balance typically formulated for each component of a system separately. A cost balance applied to the j^{th} component shows that the sum of cost rates accompanying all exiting exergy streams equals the sum of cost rates of all entering exergy streams plus the appropriate charges due to capital investment and O&M expenses. Accordingly, for a component receiving a heat transfer and generating power it gives

$$\sum_{e} \dot{C}_{e,j} + \dot{C}_{\dot{W},j} = \dot{C}_{\dot{Q},j} + \sum_{i} \dot{C}_{i,j} + \dot{Z}_j \qquad (2.3)$$

This latter equation states that the total cost of the exiting exergy streams equals the total cost of the entering exergy streams plus the capital and other costs. When a component receives power the term of cost rate associated with it would change position in the balance moving at the second member of the equation, vice versa for the cost rate associated with a heat transfer from the component, so that cost balances are generally written with all positive terms. Introducing the cost rate expressions in Equation (2.3), it becomes

$$\sum_{e} \left(c_e \, \dot{\mathbf{E}}_e \right)_j + \left(c_{\dot{W}} \, \dot{W} \right)_j = \left(c_{\dot{Q}} \, \dot{\mathbf{E}}_{\dot{Q}} \right)_j + \sum_{i} \left(c_i \, \dot{\mathbf{E}}_i \right)_j + \dot{Z}_j$$

An exergy analysis conducted at a previous stage has the aim to calculate the exergy rates exiting and entering the j^{th} component present in the equation. The cost rate of investment and O&M associated with j^{th} component are calculated considering all the costs over their lifetime i.e. computing the levelized values of these ones per unit of time, normally per hour, of system operation. The variables c are the levelized costs per unit of exergy for the exergy streams associated with the j^{th} component. Analyzing a component, it is possible to assume that the costs per exergy unit are known for all entering streams into the components in question, by the purchase cost of this stream. Consequently, the unknown variables are those ones per exergy unit of the exiting material streams and, if power or useful heat are generated in that component, the cost per unit of exergy associated with the transfer of power or heat; namely the specific *costs of products* knowing those of the fuels.

2.1.1. Applying exergy costing with fuel and product approach

The productive purpose of a component in an overall production process measured in economic terms or in terms of exergy can be called product. To create this product, one, or more than one, economic or exergy flow is consumed, such a flow can be called fuel of that component. This is what is called *fuel-product viewpoint* [14].

The *level* at which the cost balances are formulated affects the results of a thermoeconomic assessment. When *information* is not sufficient, it is preferable to make appropriate assumptions not to consider groups of components but to applicate exergy costing at the component level. Depending on the component, it can even be appropriate to distinguish among the various processes taking place within the same component. Considering only the aggregated system, it often happens not to take into account important information related to the actual production process and, thus, to the actual cost formation within the system.

The product is defined according to the *purpose* of owning and operating the component in question and the fuel represents the resources expended in generating the product, both the product and the fuel are expressed in terms of exergy. For example, for a heat exchanger the rate of exergy stream of fuel is given by the decrease in exergy rate from the side of the hot fluid and the rate of exergy stream of product is given by the increase in exergy rate from the side of the cold fluid. The product and fuel are identified with

$$\dot{\mathbf{E}}_{C,out} - \dot{\mathbf{E}}_{C,in} \;; \quad \dot{\mathbf{E}}_{H,in} - \dot{\mathbf{E}}_{H,out}$$

where the subscript $C, in/out$ and $H, in/out$ stand for the cold and hot flows in the exchanger, respectively. The associated cost rates are then

$$\dot{C}_P = \dot{C}_{C,out} - \dot{C}_{C,in} \;; \quad \dot{C}_F = \dot{C}_{H,\mathrm{in}} - \dot{C}_{H,\mathrm{out}}$$

respectively. The cost rate balance then reads an equation that can be expressed also in terms of the fuel and product cost rates

$$\dot{C}_{C,out} + \dot{C}_{\mathrm{H,out}} = \dot{C}_{C,in} + \dot{C}_{\mathrm{H,in}} + \dot{Z}$$

$$\left(c\,\dot{\mathbf{E}}\right)_{C,out} - \left(c\,\dot{\mathbf{E}}\right)_{C,in} = \left(c\,\dot{\mathbf{E}}\right)_{H,in} - \left(c\,\dot{\mathbf{E}}\right)_{H,out} + \dot{Z}$$

where the only unknowns are $c_{C,out}$ and $c_{H,out}$ since the outflows are not known. The heat exchanger removes exergy from the hot stream to heat the cold one, so the average specific cost for the hot stream remains constant and is equal to the average cost at which each exergy unit of hot stream entering the component was supplied in upstream components. Accordingly, knowing $c_{H,out} = c_{H,in} = c_H$ the last unknown may easily be estimate

$$c_{C,out} = \frac{\left(c\,\dot{\mathbf{E}}\right)_{C,in} + c_H\left(\dot{\mathbf{E}}_{H,in} - \dot{\mathbf{E}}_{H,out}\right) + \dot{Z}}{\dot{\mathbf{E}}_{C,out}}$$

The stream that leaves the heat exchanger at the cold side bears the full burden of the costs associated with owning and operating the heat exchanger, if, instead, the purpose of the component is to provide cooling, the stream outgoing at the hot side is then burdened with all costs associated with the heat exchanger. Bejan et al. [4] highlight some general principles applied in the formulation of auxiliary relations, such as that used in the example to use a single specific cost at the hot side of the heat exchanger:

- when the product definition involves a single exergy stream, the unit cost of this stream is evaluated from the cost balance. The auxiliary relations are formulated for the remaining exiting exergy streams used in the definition of fuel or in the definition of exergy loss;
- when the product definition for a component involves n exiting exergy streams, $n-1$ auxiliary relations referring to these product streams must be formulated. In the absence of information, it can be assumed that each unit of exergy is supplied to each product stream at the same average cost;
- when the fuel definition for a component involves the difference between the entering and the exiting states of the same stream of matter, the average cost per exergy unit remains constant for this stream.

It is possible to define the average costs per exergy unit of fuel and product

$$c_{\mathrm{F},j} = \frac{\dot{C}_{\mathrm{F},j}}{\dot{\mathbf{E}}_{\mathrm{F},j}} \quad ; \quad c_{\mathrm{P},j} = \frac{\dot{C}_{\mathrm{P},j}}{\dot{\mathbf{E}}_{\mathrm{P},j}}$$

The *average unit cost of the fuel* expresses the average cost at which each unit of fuel is supplied to the j^{th} component and, dually, the *average unit cost of the product* is the average cost at which each exergy unit of the product of the j^{th} component is generated.

2.1.2. Cost of exergy loss and destruction

The cost rate associated with exergy loss represents the monetary loss associated with the waste of exergy from a system to its surroundings. The loss might consist of exergy loss associated with heat transfer to the surroundings, streams of matter rejected to the surroundings and not further used within the overall system being analysed or in another system. Using the cost rates associated with fuel and product as shown before, the cost rate balance becomes

$$\dot{C}_{\mathrm{P},j} = \dot{C}_{\mathrm{F},j} - \dot{C}_{\mathrm{los},j} + \dot{Z}_j$$

$$\left(c\,\dot{\mathbf{E}}\right)_{\mathrm{P},j} = \left(c\,\dot{\mathbf{E}}\right)_{\mathrm{F},j} - \dot{C}_{\mathrm{los},j} + \dot{Z}_j \qquad (2.4)$$

The cost rate of the *exergy loss* stream $\dot{C}_{los}$ affects evidently the cost rate associated with the product of the component.

When such cost rate is *zero* the product bears the full burden of the costs associated with owning and operating the j^{th} component. Such a case is useful when the purpose of the thermoeconomic analysis is to estimate the costs of the final products or to calculate or optimize the overall system and it should be applied only to streams finally discharged to the natural environment. When the purpose of the analysis is, instead, to understand the cost formation process and the cost flow in the system, to know the performance of a single component, or to optimize specific design variables in a component, all exergy loss streams should be cost as if they were to be further used by the system. This way the cost rate of loss equals the product of the average specific cost of fuel multiplied by the exergy loss rate: exergy loss is covered through the supply of *additional fuel* to the j^{th} component and the average cost of supplying the fuel exergy unit remains constant with varying exergy loss. If it is assumed that the exergy loss results in a *reduction of the exergetic product* and that the average cost of generating the product remains practically constant with varying exergy loss in the j^{th} component, the monetary loss associated with the exergy loss is given by the product of the average specific cost of product multiplied by the exergy loss rate. As this approach overestimate the cost penalty associated with exergy loss, it is not recommended for any analysis.

In general, very few components have exergy losses that need to be distinguished from the exergy destructions for costing purpose. The concept of exergy loss is applicable to the *overall system* rather than to a single component usually. A component should not penalized for a loss, particularly if the exiting stream has been used in more than one component or it is leaving the overall system with the lowest allowable temperature, pressure and chemical exergy values.

The presence, during a generic process, of irreversibilities, that can be computed by estimating the generation of entropy, causes the duty to consider the existence of a quantity of exergy destruction. The latter brings with it a hidden cost very important that can be revealed only through a thermoeconomic analysis. The effect of *exergy destruction* can be demonstrated with the exergy balance for a j^{th} component

$$\dot{\mathbf{E}}_{\mathrm{F},j} = \dot{\mathbf{E}}_{\mathrm{P},j} + \dot{\mathbf{E}}_{\mathrm{los},j} + \dot{\mathbf{E}}_{\mathrm{des},j}$$

in a fuel and product logic. By combining such balance with Equation (2.4) and eliminating the exergy rate of fuel or product, it obtains

$$\left(c\,\dot{\mathbf{E}}\right)_{\mathrm{P},j} = c_{\mathrm{F},j}\,\dot{\mathbf{E}}_{P,j} + \left(c_{\mathrm{F},j}\,\dot{\mathbf{E}}_{\mathrm{los},j} - \dot{C}_{\mathrm{los},j}\right) + \dot{Z}_j + c_{\mathrm{F},j}\,\dot{\mathbf{E}}_{\mathrm{des},j} \tag{2.5}$$

$$c_{\mathrm{P},j}\,\dot{\mathbf{E}}_{\mathrm{F},j} = \left(c\,\dot{\mathbf{E}}\right)_{\mathrm{F},j} + \left(c_{\mathrm{P},j}\,\dot{\mathbf{E}}_{\mathrm{los},j} - \dot{C}_{\mathrm{los},j}\right) + \dot{Z}_j + c_{\mathrm{P},j}\,\dot{\mathbf{E}}_{\mathrm{des},j} \tag{2.6}$$

The last term at the second member involves the rate of exergy destruction in each of equations, these terms provide measure of the *cost of exergy destruction*. Assuming that the exergy rate of the product is fixed and that the specific cost of fuel of the j^{th} component is independent of the exergy destruction, the cost of exergy destruction can be written as

$$\dot{C}_{\mathrm{des},j} = c_{\mathrm{F},j}\,\dot{\mathbf{E}}_{\mathrm{des},j}$$

Such a cost may be interpreted as the cost rate of the *additional fuel* that must be supplied to the j^{th} component, over and above the rate needed for the product, to cover the rate of exergy destruction because the fuel exergy rate must account for the fixed product exergy rate and the rate of exergy destruction. Alternatively the cost rate can be defined using the specific cost of product, dually, so cost rate of exergy destruction may be interpreted as the monetary loss associated with the *loss of product*. Really neither of the sets of assumptions used to define the cost rate is strictly satisfied and these correlations are just approximations of the average costs rate associated with exergy destruction in the j^{th} component. The use of the specific cost of fuel or of product, for most applications, respectively gives a lower or a higher estimate with the actual exergy destruction cost *being somewhere between the two*.

Exergy destruction affects directly the capital investment for the component and, in some cases, indirectly affects the capital investment and the fuel costs of other component in well-designed systems. As the exergy destruction decreases or as the efficiency increases, the cost rate of the exergy destruction decreases, but the capital investment increases. The design optimization of a single component in isolation consists of finding the appropriate trade-offs between the cost of exergy destruction and the cost of investment that minimize the unit cost of the product generated in the component. The lower the specific cost used to evaluate cost rate of exergy destruction, the lower the cost optimal value of the investment. Using specific cost of fuel represents a *prudent approach* with the required capital investment costs. This is consistent with *common practice* in the design of industrial system [15]. Moreover, considering the term linked to the rate of exergy loss and its cost, as said, the simplest approach to costing it is to set it equal to zero: since this assumption is consistent with the purpose of evaluating and optimizing the design of a system, it is possible to assume that such a condition applies in the derivation of the other thermoeconomic variables. Expressing the cost rate of the loss using specific cost of product or of fuel lead to a zero value of the term linked to the rate of exergy loss and its cost in the previous balances (Equations (2.5) or (2.6)), thus no exergy loss cost would be charged to the average unit cost of the product of the j^{th} component.

2.1.3. Design and performance evaluations

Two important thermoeconomic variables used in evaluating systems are the relative cost difference and the exergoeconomic factor. The *relative cost difference* for the j^{th} component is defined by the equation

$$r_j = \frac{c_{P,j} - c_{F,j}}{c_{F,j}} \tag{2.7}$$

Such a variable expresses the relative increase in the average cost per exergy unit between fuel and product of the component. This relative difference is useful to evaluate and to optimize a system component. In an iterative cost optimization of a system if, for example, the cost of fuel of a major component changes from one iteration to the next, the objective of the cost optimization of the component should be to minimize the relative cost difference instead of minimizing the cost per exergy unit of the product for this component. With Equations (2.2) and (2.5) and by considering a zero cost rate of exergy loss, Equation (2.7) becomes

$$r_j = \frac{c_{\mathrm{F},j}\left(\dot{\mathbf{E}}_{\mathrm{des},j} + \dot{\mathbf{E}}_{los,j}\right) + \left(\dot{Z}_j^{CI} + \dot{Z}_j^{O\&M}\right)}{c_{\mathrm{F},j}\,\dot{\mathbf{E}}_{\mathrm{P},j}} \tag{2.8}$$

revealing the actual cost sources associated with the j^{th} component. The sources that cause an increase in the cost per exergy unit between fuel and product are, this way, the cost rates associated with the capital investment, O&M, exergy destruction and loss. Introducing the exergetic efficiency of the j^{th} component, Equation (2.8) can be rewritten

$$\eta_{exe,j} = \frac{\dot{\mathbf{E}}_{\mathrm{P},j}}{\dot{\mathbf{E}}_{\mathrm{F},j}} = 1 - \frac{\dot{\mathbf{E}}_{\mathrm{des},j} + \dot{\mathbf{E}}_{los,j}}{\dot{\mathbf{E}}_{\mathrm{F},j}}$$

$$r_j = \frac{1-\eta_{exe,j}}{\eta_{exe,j}} + \frac{\dot{Z}_j^{CI} + \dot{Z}_j^{O\&M}}{c_{\mathrm{F},j}\,\dot{\mathbf{E}}_{\mathrm{P},j}} \tag{2.9}$$

Equation (2.8) and (2.9) show the contribution of the exergy destruction and loss in the assessment of the relative cost difference indicating that the cost sources in a component may be grouped in two categories.

In evaluating the performance of a component, it is interesting to know the relative importance of non-exergy-related costs that related to exergy destruction and loss. The *exergoeconomic factor* provide such an information being defined, for a j^{th} component as

$$f_j = \frac{\dot{Z}_j}{\dot{Z}_j + c_{\mathrm{F},j}\left(\dot{\mathbf{E}}_{\mathrm{des},j} + \dot{\mathbf{E}}_{los,j}\right)}$$

The denominator gives the total cost rate causing the increase in the unit cost from fuel to product. Hence, the exergoeconomic factor expresses as a ratio the contribution of the non-exergy-related cost to the total cost increase. A low value of this factor calculated for a major component suggests that cost savings in the entire system might be achieved by improving the component efficiency, reducing exergy destruction, even if the capital investment for this component will increase. Dually, a high value of the exergoeconomic factor suggests a decrease in the investment costs of this component at the expense of its exergetic efficiency. Typical values of the factor depend on the component type, lower than 55% for heat exchangers, between 35 and 75% for compressors and turbines and above 70% for pumps.

The *design evaluation* is based on a set of variables calculated for each component of the system. It is thus fundamental to evaluate the exergetic efficiency, the rates of exergy destruction and loss, the cost rates associated with capital investment and O&M, the cost rate of exergy destruction and the relative cost difference with the exergoeconomic factor. To enhance the cost effectiveness of a thermal system consisting of several components, it needs:

1. to rank the components in descending order of cost importance considering *the sum of cost rate of investment and the cost rate of exergy destruction*;
2. to consider *design changes* for the components for which the value of such sum is high;
3. to pay attention to components with a high *relative cost difference*, especially when the sum referred to in point 1 is high;
4. to use the *exergoeconomic factor* to identify the major cost source between the cost rate of investment and the cost rate of exergy destruction; if the value of the factor is high it must be investigated whether it is cost effective to reduce the capital investment for the component at the expense of the efficiency, if the factor is low, instead, it must be improved the component efficiency by increasing the capital investment;
5. to eliminate any subprocesses that increase the *exergy destruction* or loss without contributing to the reduction of *capital investment* or of fuel costs for other components;
6. to consider improving the *exergetic efficiency* of a component if it has a relatively low exergetic efficiency or relatively large values of the rate of *exergy destruction*.

The *performance evaluation* of an actual system is conducted in a parallel manner as the design evaluation of a new system. Capital investment is ignored as it represents a sunk cost. Furthermore, for simplicity it is possible to neglect the effect of the O&M cost so that only the fuel cost is considered and the exergoeconomic factor vanishes. Selected thermoeconomic variables can be used to help to understand the effects of a malfunction in a component on the performance of the other components and the total system; the values of the variables can so be compared with design or target values to check their performances, detecting malfunctions and their sources. Exergy stream cost data can be used to decide whether a faulty component should be replaced.

It is moreover necessary to consider that in some systems, the *chemical and physical exergy* of streams may be supplied or generated at different unit costs. Neglecting the kinetic and potential contribution, the cost rate associated with a stream of matter is

$$\dot{C} = c\,\dot{\mathbf{E}} = \left(c\,\dot{\mathbf{E}}\right)^{ch} + \left(c\,\dot{\mathbf{E}}\right)^{ph}$$

a cost rate that is so associated with the total exergy of the stream. The cost per unit of chemical exergy of a stream remains constant when the chemical composition does not change, for example, in a case of a complete combustion in a combustion chamber of a boiler, a zero cost is assigned to the chemical exergy of the combustion products as such a exergy cannot be retrieved by practical means, but if combustion is incomplete the specific cost of chemical exergy is set equal to the specific cost of fuel chemical exergy. In some other application it is also possible and appropriate to further divide each of the chemical and physical contributions into terms of subcontributions which are costed individually.

2.1.4. Input-Output method

So far, the thermoeconomic analysis has been presented in the traditional manner; the thermoeconomic algebraic system, made so as to engage the exergy rates balance and cost rates balance with the allocation of costs on exergetic basis, according to the state of the art, may be solved by borrowing from economics the methodology of the *Input-Output analysis* which uses the matrixes. An approach of this kind can be very handy when it needs to write complicated algebraic systems while considering many processes or components of a plant. This method has been developed starting from the tables of national economy but this does not prevent the application of such a method to a narrower level, as the regional one or even to the study of a real thermodynamic system or a plant in particular, provided that the Input-Output matrix for the analysis is properly constructed.

The *Input-Output table of a national economy* is a square matrix summarising the commodities (inputs or fuels) necessary to make other commodities (outputs or products) [2]. For a given set of outputs the direct inputs required can be found through matrixes calculations. The result of this analysis is a list of all the commodities required, within the nation covered by the

Input-Output table, to produce a specified output. The table cannot be broken down into individual firms but have to deal with industries in groups. This can lead to errors if the commodities are liable to large price fluctuations or if some purchasers can obtain special prices for them. Another disadvantage is that the method deals with transactions in financial terms, not in terms of physical quantities.

Leontief's original Input-Output framework conceived of industry production functions, which he frequently referred to as production "recipes", as measured in *physical units*, such as tons of coal or bushels of wheat, as inputs, required per ton of steel output or per 1 € worth of an industry output [16]. However, the data collection requirements and other constraints rendered implementation of the framework in physical units too heavy, so, the basic methodology for Input-Output analysis evolved through measuring all quantities in value terms with implicit fixed prices. All the researchers contributions have extended the Input-Output framework incrementally in the direction of employing physical units helping to lay the groundwork for new research areas such as industrial ecology and ecological economics, especially where public policies have encouraged such developments and data have been collected easily. Accordingly, the analysis provides useful framework for tracing energy use and other related characteristics such as *exergy* or other environmental indicators. The generalization of this techniques to a much broader conceptual level, such as accounting for social indicators, began with simpler attempts to link Input-Output accounting techniques with many measurable quantities, such as energy use, therefore exergy, environmental pollution or employment.

In all instances the Input-Output approach is essentially the same. The structure of each process is represented by an appropriate vector of structural coefficients that describes in quantitative terms the relationship between the inputs it absorbs and the output it produces (*Leontief's production model*) [17]. The interdependence among the processes of a system is described by a set of linear equations expressing the balances between the total input and the aggregate output of each commodity and service produced and used in the course of one or several periods of time. Such a technical structure can accordingly be represented by the matrix of technical Input-Output coefficients of all the processes of the system. An *Input-Output table* describes the flow of goods between all the individual components of a system, or the sectors of an economy, over a stated period of time. A simplified example of a table depicting n processes of a system is described in Table 2.1. Each element x_{ij} represents the output for the process i which is an input for the process j. The goods are produced by using the resources from the outside, given, for each process, by v_i.

		Process (x_{ij})				Final demand (y_i)	Total (x_i)
		1	2	…	n		
Process	1	x_{11}	x_{12}	…	x_{1n}	y_1	x_1
	2	x_{21}	x_{22}	…	x_{2n}	y_2	x_2
	…	…	…	⋱	…	…	…
	n	x_{n1}	x_{n2}	…	x_{nn}	y_n	x_n
Exogenous rosources (v_i)		v_1	v_2	…	v_n		

Table 2.1 – Simplified Input-Output table for a system with n processes

The elements y_i are the actual products of the system to the outside, they constitute the final demand of the environment to the system. For each process, each element x_i, represents, instead, the *total output* composed by the sum of the outputs of that process for other processes within the system and to the outside as expressed by the equation

$$x_i = \sum_{j=1}^{n} x_{ij} + y_i \tag{2.10}$$

Through a quantitative analysis the vector $\boldsymbol{x}$ (composed by the x_i) of the total outputs may be estimated. This can be done by considering that the quantity of the output of process *i* absorbed by process *j* per unit of total output *j* may be described by the *technical coefficient* a_{ij} i.e. the input coefficient of product of sector *i* into sector *j*

$$a_{ij} = \frac{x_{ij}}{x_j} \tag{2.11}$$

A complete set of the technical coefficients of all processes of a system arranged in the form of a *rectangular table* is the structural *matrix* of that system, $\boldsymbol{A}$. Similarly can be defined a *vector of the specific* (per unit of total output) *exogenous resources* whose components are defined by

$$b_i = \frac{v_i}{x_j} \tag{2.12}$$

So, Equation (2.10) can be rewritten as

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

$$\boldsymbol{x} = \boldsymbol{A}\,\boldsymbol{x} + \boldsymbol{y}$$

where the second expression considers directly the involved matrixes. Since $\boldsymbol{A}$ is a *non-singular invertible matrix*, the vector of the total outputs may be evaluated by using the *Leontief inverse* $(\boldsymbol{I} - \boldsymbol{A})^{-1}$ where $\boldsymbol{I}$ is the identity or unit matrix of size n with ones on the main diagonal and zeros elsewhere. Both $\boldsymbol{A}$ and $\boldsymbol{I}$ are *square matrixes* $(n \times n)$. Vector $\boldsymbol{x}$ is then expressed by

$$\boldsymbol{x} = \left(\boldsymbol{I} - \boldsymbol{A}\right)^{-1} \boldsymbol{y}$$

In *Leontief's cost model*, from *economics*, the *concept of cost* is introduced and it appears that the cost of a good may be expressed by a *specific cost* multiplied by the quantity of the output considered. Unit cost (per unit of total output) of each process is equal to the unit cost of each output of that particular process, hence, it results

$$c_i = c_{i1} = \ldots = c_{in}$$

Therefore a *cost balance* may be written as

$$c_i\, X_i = \sum_{j=1}^{n} c_j\, X_{ji} + V_i \qquad (2.13)$$

considering the exogenous resources in the same units of costs. *Unit costs* of each process can be evaluated merging Equations (2.11) and (2.12) with Equation (2.13)

$$c_i = \frac{\sum_{j=1}^{n} c_j\, X_{ji} + V_i}{X_i}$$

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

By switching to *matrix notation* it is finally possible to solve the problem, as done previously

$$\boldsymbol{c} = \boldsymbol{A}^T\, \boldsymbol{c} + \boldsymbol{b}$$

$$\boldsymbol{c} = \left(\boldsymbol{I} - \boldsymbol{A}^T\right)^{-1} \boldsymbol{b} \tag{2.14}$$

The transpose of the matrix $\boldsymbol{A}$ takes place considering the reversal of subscripts in the technical coefficients as defined by cost balance.

When considering a thermal plant it is imaginable to think that every process happens in a specific *component* or set of components of a examined system, so the word 'process' can be replaced by that of the component in which it occurs.

2.1.5. Exergy based Input-Output matrix

The two concept to bear in mind during a thermoeconomic analysis are exergy cost and purpose. *Exergy cost* of a flow is the amount of exergy needed to produce it. Matter and energy flows entering and exiting a given component have to be classified into *fuel and product*. For performing thermoeconomic analysis, the physical structure of an assessed thermodynamic system, where all physical flows appear, has to be substituted by a productive structure, where fuel and product flows are depicted [18]. Thermoeconomic Input-Output analysis based on matrix notation, can be easily implemented in computers. All components of a system are numbered starting from 1 to n, and the number 0 corresponds to the environment. The element $\mathbf{E}_{ij}$ represent the exergy rate that is an output for the component i and becomes an input for the component j. Accordingly, the *exergy Input-Output matrix* can be constructed, together with the vector of the outputs to the environment and the vector with the inputs, by

$$\begin{array}{c|cccc|c} & 1 & 2 & \cdots & n & 0 \\ \hline 1 & \mathbf{E}_{11} & \mathbf{E}_{12} & \cdots & \mathbf{E}_{1n} & \mathbf{E}_{10} \\ 2 & \mathbf{E}_{21} & \mathbf{E}_{22} & \cdots & \mathbf{E}_{2n} & \mathbf{E}_{20} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ n & \mathbf{E}_{n1} & \mathbf{E}_{n2} & \cdots & \mathbf{E}_{nn} & \mathbf{E}_{n0} \\ \hline 0 & \mathbf{E}_{01} & \mathbf{E}_{01} & \cdots & \mathbf{E}_{0n} & \end{array}$$

An exergetic cost balance will be verified for any component to represent that the exergetic cost of the product has to be equal to that of the needed resource [19]. The square matrix which considers the exergy rates of the n

components of the system is the *fuel-product exergy table* or else exergy Input-Output matrix

$$\boldsymbol{E} = \begin{pmatrix} \mathbf{E}_{11} & \cdots & \mathbf{E}_{1n} \\ \vdots & \ddots & \vdots \\ \mathbf{E}_{n1} & \cdots & \mathbf{E}_{nn} \end{pmatrix}$$

The *vector of the outputs to the environment* is constructed considering only the exergy flows accompanying products that represent the actual commodities engendered by the production system under consideration, it can be represented as

$$\boldsymbol{y}_{env}^{T} = \begin{pmatrix} \mathbf{E}_{10} & \cdots & \mathbf{E}_{n0} \end{pmatrix}$$

where the transposition is drafted to be consistent with the previous presentation of the vector. It can be seen as the vector of the *final demand* of the environment to the system. The *vector* that represents, instead, the *inputs coming from the environment* to the system, may also be indicated as the *exogenous resources vector* and it can be represented as

$$\boldsymbol{v}_{env} = \begin{pmatrix} \mathbf{E}_{01} & \cdots & \mathbf{E}_{0n} \end{pmatrix}$$

When the resource comes from the environment through the control volume of the system, its cost equals its exergy: the exergy that was needed to produce it is an external cost, which does not affect the system under study. Two other vectors can be constructed considering the sums

$$x_i = \sum_{j=0}^{n} \mathbf{E}_{ij}$$

$$w_j = \sum_{i=0}^{n} \mathbf{E}_{ij}$$

for each i^{th} or j^{th} component (it is the same because i and j ranging from 1 to n represent all components respectively by row or by column) it is possible to evaluate the *total fuel and product utilized and generated*. Hence, the *vector of the total products* produced by each component and by the system as a whole is

$$\boldsymbol{x}^{T} = \begin{pmatrix} x_1 & \cdots & x_n \end{pmatrix}$$

It can be seen as the vector of the total output. Similarly the *vector of the total inputs* used as fuels by each component of the system and from the environment is

$$\boldsymbol{w} = \begin{pmatrix} w_1 & \cdots & w_n \end{pmatrix}$$

By using the Leontief's procedure, coherently to Equation (2.11), the *technical coefficients matrix* can be evaluated through the expression

$$\boldsymbol{A} = \boldsymbol{E}\left[diag\left(\boldsymbol{x}\right)\right]^{-1} \tag{2.15}$$

which involves the exergy Input-Output matrix and the vector of total products already defined and which is an invertible, or rather non-singular, square matrix ($n \times n$) [20]. Such a construction constitutes the basis to calculate the specific costs of products and fuels for the various components and for the whole system as well as the parameters of the exergoeconomic analysis, namely for performing the *thermoeconomic Input-Output analysis*.

2.2. Exergy cost analysis

The thermoeconomic Input-Output analysis can be carried out first of all studying the *exergetic cost* of the material and energetic flows among the components of a thermodynamic system. Without involving economic information, since the matrix regarding the exergy flows exchanged between the components and the environment has been constructed, it is possible to estimate the *specific costs* of products and fuels such as the exergy required to produce 1 J of exergy of product or fuel and also *cost rates* (e.g. of products or of exergy destruction) as exergy required per unit of time.

2.2.1. Exergy Input-Output analysis

The *exogenous resources vector* consists of exergy flows, in particular,

$$v_{env,j} = \dot{\mathbf{E}}_{0\mathrm{j}}$$

Thus the *exergetic specific exogenous resources vector*, coherently to Equation (2.12), is estimated as

$$\boldsymbol{b}_{exe} = \boldsymbol{v}_{env} \left[diag\left(\boldsymbol{x}\right) \right]^{-1}$$

involving the vector of total products. Accordingly, by following Equation (2.14), it is possible to calculate the *specific exergetic cost vector of product* per unit of exergy from the equation

$$\boldsymbol{c}_{exe,P} = \left(\boldsymbol{I} - \boldsymbol{A}^T\right)^{-1} \boldsymbol{b}_{exe}$$

The vector is composed of n specific costs, one for each component, expressed in J/J (or kWh/kWh) representing the *exergetic expense* to produce 1 J (or 1 kWh) of exergy accompanying the output flow of the considered component.

The *rate of exergy destruction* can be evaluated from the balance between inputs and outputs of the system combined with the environment: the *vector* of the rates for each component is determined by

$$\boldsymbol{E}_{des} = \boldsymbol{w} - \boldsymbol{x}^T$$

where the transposition is worded to be consistent with the previous expressions. By using the terms of this simple balance it is then possible to estimate the *exergetic efficiency* of each component arranged in the efficiency *vector*

$$\boldsymbol{\eta}_{exe} = \frac{\boldsymbol{x}^T}{\boldsymbol{w}}$$

and so the *exergy specific cost of fuel vector* by

$$\boldsymbol{c}_{exe,F} = \boldsymbol{c}_{exe,P}\, \boldsymbol{\eta}_{exe}$$

The latter expresses the array of *exergy specific costs of needed resources* for each component of the system expressed in J/J (or kWh/kWh) and representing the exergetic expense to produce 1 J (or 1 kWh) of exergy accompanying the input flow of the considered component. Finally, the *exergy cost rate of the product* (dually may be evaluated that of the fuel) can be calculated considering the rate cost, product by product for each component or considering the whole system output. In the first case it can be estimate according to the *vector* expression

$$\boldsymbol{C}_{exe,P} = \boldsymbol{c}_{exe,P}\, \boldsymbol{x}^{T}$$

thus, each component is associated to a cost rate in kW that stands for the expense in kJ made to produce an output from the component per every second. If the intention of the analysis is, instead, that to highlight the cost rate of the *total system as a whole*, the vector has to be referred only to the outputs that represent an actual product of the system instead of considering the total output of each component

$$\boldsymbol{C}^{SY}_{exe,P} = \boldsymbol{c}_{exe,P}\, \boldsymbol{y}^{T}_{env}$$

The components of such a vector may be summed to obtain the *total exergy cost rate of the system*

$$\dot{C}^{SY}_{exe,P\,tot} = \sum_{i} C^{SY}_{exe,P,i}$$

where the term at first member is the sought element in kW and the terms of the summation at the second member are the components of the vector $\boldsymbol{C}^{SY}_{exe,P}$: for i ranging from 1 to n all terms are zero except for those components of the system that produce the real products.

2.2.2. Thermoeconomic variables

In an exergy thermoeconomic Input-Output analysis may be evaluated, in agreement with the thermoeconomic theory outlined, the *overall exergetic efficiency* as

$$\eta^{SY}_{exe} = \frac{\sum_{i} \mathbf{E}_{i0}}{\sum_{i} \mathbf{E}_{0i}}$$

in which the total exergetic contributions of products and fuels (exogenous resources) to and from the environment are considered. The *exergy cost rate of exergy destruction* in kW can be evaluated as a vector by

$$\boldsymbol{C}_{exe,\mathrm{des}} = \boldsymbol{c}_{exe,\mathrm{F}}\,\boldsymbol{E}_{\mathrm{des}}$$

The terms in such an array represent, for each component, the *exergetic cost* rate in kJ of the *additional fuel*, that must be supplied to the component to cover the rate of exergy destruction due to irreversibilities, per unit time. Alternatively the cost rate can be defined using the vector of specific cost of product dually, and so it may be interpreted as the exergetic loss associated with the loss of product. At last, also the *relative cost difference* can be estimated using Equation (2.7), about it all the considerations made are valid, but in such a case the terms $\boldsymbol{c}_{exe,P}$ and $\boldsymbol{c}_{exe,F}$ are expressed as vectors.

2.3. Exergoeconomic cost analysis

The thermoeconomic Input-Output analysis can be, then, carried out estimating the *economic cost* of the flows in the system under analysis. Economic information is introduced through the use of a new exogenous resources vector but the calculation procedure amongst matrixes remains the same of the exergy Input-Output analysis. The *specific costs* of products and fuels such as the monetary resources required to produce 1 € worth of exergy of product or fuel and also *cost rates* as euro per unit of time are evaluated together with *variables for the design analysis* as the exergoeconomic factor.

2.3.1. Exergoeconomic Input-Output analysis

By using Equation (2.15) the technical coefficient matrix has been calculated as a non-singular square matrix $(n \times n)$. The economic exogenous resources vector is constructed considering or better adding, for each component, the *cost rates of fuels*, of *capital investment* and *O&M* expressed as euro per unit of time, typically hours

$$v_{eco,j} = \dot{C}_{f,j} + \dot{Z}_j^{CI} + \dot{Z}_j^{O\&M}$$

The *specific exogenous resources vector* is, so, defined on economic basis as

$$\boldsymbol{b} = \boldsymbol{v}_{eco}\left[diag\left(\boldsymbol{x}\right)\right]^{-1}$$

similarly to the vector $\boldsymbol{b}_{exe}$ in the previous paragraph. Through Leontief's inversion it is possible to calculate the *specific cost vector* per unit of product from the equation

$$\boldsymbol{c}_P = \left(\boldsymbol{I} - \boldsymbol{A}^T\right)^{-1} \boldsymbol{b}$$

The vector is composed of n specific costs, one for each component, expressed in €/kWh representing the *economic expense* to produce 1 kWh of exergy accompanying the output flow of the considered component. Dually, the *cost rate of the products* can be calculated considering the rate cost, product by product, according to the vector expression

$$\boldsymbol{C}_P = \boldsymbol{c}_P \, \boldsymbol{x}^T$$

thus each component is associated to a cost rate in €/h that stands for the monetary expense incurred to produce an output from the component every hour. This way, considering the balance of Equations (2.1) and (2.2) but referred to each component, the *cost rate vector of the fuels* (exergetic flows) can be evaluated via

$$\boldsymbol{C}_F = \boldsymbol{C}_P - \boldsymbol{Z}$$

where the vector $\boldsymbol{Z}$ is composed by the costs of capital investment and O&M of each component. Hence, the *specific cost vector of fuel* can be calculated by

$$\boldsymbol{c}_F = \frac{\boldsymbol{C}_F}{\boldsymbol{w}}$$

The latter expresses the array of specific costs of needed resources for each component of the system in €/kWh and representing the economic expense to produce 1 kWh of exergy accompanying the input flow of the considered component.

If the intention of the analysis is, instead, that to show the *cost rate of the total system* as a whole, the vector $\boldsymbol{C}_P$ has to be referred only to the outputs that represent an actual product of the system, instead of considering the total output of each component, that is

$$\boldsymbol{C}_P^{SY} = \boldsymbol{c}_P \, \boldsymbol{y}_{env}^T$$

The components of such a vector can be added to obtain the *total cost rate of the products of the system*

$$\dot{C}^{SY}_{P\,tot} = \sum_i C^{SY}_{P,i}$$

where the term at first member is the required rate in €/h and the terms of the summation at the second member are the components of the vector $\boldsymbol{C}^{SY}_{P}$: for i ranging from 1 to n all terms are zero except for those components of the system that produce the real products. By knowing the amount of the total investment costs rate in €/h it is possible to estimate by difference the *total cost rate of the fuels* of the system since

$$\dot{C}^{SY}_{P\,tot} = \dot{C}^{SY}_{F\,tot} + \dot{Z}^{SY}_{tot}$$

2.3.2. Thermoeconomic variables

In an exergoeconomic Input-Output analysis can be evaluated, in agreement with the thermoeconomic theory outlined, the *cost rate of exergy destruction vector* in euro per unit of time by

$$\boldsymbol{C}_{\mathrm{des}} = \boldsymbol{c}_{\mathrm{F}}\, \boldsymbol{E}_{\mathrm{des}}$$

The terms in such an array represent, for each component, the cost rate in € of the additional fuel, that must be supplied to the component to cover the rate of exergy destruction due to irreversibilities, per unit time. Alternatively, the cost rate can be defined using the vector of specific cost of product, this way it may be interpreted as the economic loss associated with the loss of product. By using Equation (2.7) the relative cost difference can be calculated with the terms $\boldsymbol{c}_P$ and $\boldsymbol{c}_F$ expressed as vectors. Also the *exergoeconomic factor* can be calculated, by considering *the sum of the costs rate of exergy destruction and investment* (that is considered another thermoeconomic variable) the factor results

$$f_i = \frac{Z_i}{C_{des,i} + Z_i}$$

where with i all the n components of the analysed system are considered.

3. Uncertainties in Thermoeconomic Input-Output Analysis

The *variability* of the data constitutes their *aptitude to occur in many different modes* [1]. In the models utilized to describe engineering problems, the variability is explained by the fact that successive observations of a system, of a phenomenon, or the change in the assumptions used in a model, do not produce exactly the same result. The *data* are almost always a selected *sample* from some population, generally, they are collected through:

- a *retrospective study*, that uses all historical data related to a specific period of time, or their sample. Using previously collected data has the advantage of minimizing the cost of data gathering, nevertheless, this involves some problems because some of the essential data may not have been collected, have been lost or have been transcribed or stored non-precisely, so highlighting issues related to their quality;
- an *observational study*, that are limited to the observation of the process or of the data population during a period of operating routine by disturbing the system only to the extent necessary to obtain the desired information unless such a study should seek information about variables that are not registered in the operating routine;
- a *planned experiment*, in which deliberate changes in the controllable variables of the system are performed to observe the resulting output, make a decision or make an inference about which variables are responsible for the observed change.

In the thermoeconomic Input-Output analysis, the variability may affect model data, collected from historical records or observed. Anyway, particular statistical techniques allow to handle *data dispersion*, and to understand how it *propagates at the results*. These will not be assumed as certain but will be accompanied by an *uncertainty interval*.

In this chapter the fundamentals about the uncertainty and its description are presented together with the methods adopted to evaluate its propagation from the input data up to the results output. In particular, a technique for the uncertainty evaluation in the thermoeconomic Input-Output analysis is provided.

3.1. Concepts and theory

Uncertainties and errors are often confused. Following the directions of metrology according to the *VIM* (International Vocabulary of Metrology) it can now shed light on these two words often used interchangeably. Next, the sources of uncertainties are listed together with the statistical approaches used to describe the data variability.

3.1.1. Error and uncertainty

The *uncertainty* is a *non-negative parameter characterizing the dispersion of the quantity values* of some data [21], it may be indicated by an *interval*, expressed by two quantities that delimit its breadth.

The measurement process can alter more or less significantly the value of an observed quantity, thus the "true value" of the quantity cannot be known. This does not invalidate the assumption of uniqueness of the measure, but it forces to estimate and express, together with the value of the quantity, the *quality of the measure*, namely the uncertainty. The non-negative parameter, characterizing the dispersion of the quantity values attributed to a quantity intended to be measured, can be expressed in absolute or relative terms.

$$x \pm u \tag{3.1}$$

Equation (3.1) represents the *absolute uncertainty*, u, which has the same units as the observed quantity, x; the *relative uncertainty* can be evaluated by dividing the value of the uncertainty by that of the quantity and it is generally expressed as a percentage.

The *measurement error* is the *difference between the measured quantity value and the reference quantity value* [21]. The "true value" of a quantity, by definition, is not known or knowable (Heisenberg uncertainty principle [22]); hence, also an error defined as the interval between the "true value" and the measured one is not known and results unknowable, therefore of no practical importance. Thus, instead of the "true value", a reference value (considered to be true conventionally) is used in order to define this error. Faced with this limit it is instead possible to obtain measurements of *the most probable value* of the studied quantity and to estimate the *range*, centred around this value, within which the reference value should fall with a certain level of confidence.

This way, it could be said that all kinds of errors are the *cause* of the data variability. The *systematic errors* is that kind of error that, in replicate measurements, *remains constant or varies in a predictable manner*, instead of *random error* that *varies in an unpredictable manner*.

3.1.2. Sources of uncertainty

All data in engineering models have some uncertainties which can be distinguished in two main types [6]:

1. *data uncertainties*;
2. *uncertainties about correctness and/or incompleteness of the model*.

Data uncertainties may be caused by systematic and random errors [23]:

- *systematic errors* are due to *defects* in materials or calibration of instruments and samples, or to *irregularities* in the experimental procedure and are related to the cause that produces them by a very *specific physics law*. Examples are errors occurring for the difference between the nominal and the real characteristic curve of a quantity, for disturbances such as crushing, thermal energy exchange, alteration of the system of currents in a circuit, pressure drops or, even, errors due to the influence of quantities such as pressure, temperature and humidity of the measurement environment. It is almost always *possible to compensate for the effects* of such biases. For example, by desensitizing the measuring instrument as for instruments for measuring length which take account of the expansion coefficient of the material or by offsetting the effects of influence, introducing a signal of equal and opposite sign to that which would be observed in the absence of compensation. Or rather, by resorting to correction of the values, when the law of dependence of the measured variable from the influence variable is known, and by using the standards that define the correct procedures to be used in order to avoid error;
- *random errors* are produced by *accidental causes* such as random irregularity of the proceedings or of the measuring instrument, *uncontrollable instability* of the environmental conditions, imperfections of the human operator or as a *result of the correction* of the systematic error. They produce a variability of aleatory nature with Gaussian distribution (see Subparagraph 3.1.3) around the mean value or with effects from time to time with different sign and different entity all equally probable. Examples of this kind of error are linked to:

- *resolution*, the ability to detect small variations of the physical quantity in question;
- *parallax*, the phenomenon in which an object appears to move relative to the background if the point of observation changes;
- *interpolation*, the construction of new data within the range of a discrete set of known observations;
- *background noise of the instrument*, an unwanted signal, natural or artificial, which overlaps the data transmitted or processed;
- *mobility*, from a state of rest to one of motion friction decreases, below a limit value a change in input does not produce an output variation;
- *inversion*, the value measured by the instrument when the quantity increases and that measured when it decreases may not match;
- *hysteresis*, the characteristic of a system to react to the stresses applied in delay and in dependence on the previous state.

Uncertainty on the correctness of the model refers to the fact that there is not just one way (a unique model) to represent the reality of the problem investigated [6]. In each engineering analysis, more or less *subjective choices* are made in order to construct a model. Some assumptions are linked to:

- *representativeness*, by considering that data used on processes of the model can come from other sources. Often, some information is missing and can be reasonably assumed from the known data or is known and is included in the analysis but it is not relevant to the phenomenon under study, therefore, errors are caused and it is difficult to assess how large the impact on the variability of results is;
- *allocation basis*, because different choices of allocation basis can be made consistent with the theory of analysis and with the cut that one wants to give to the study;
- *future events*, because many models deal with products that have a long lifetime. Thus, it is necessary to make decisions on issues that in the future could be addressed with instruments and/or knowledge which are not available today, think of the waste treatment.

Uncertainty caused by incompleteness is linked to the unavoidable *data gaps*, important issues are:

- *system boundaries*, cut-off criteria must be chosen carefully to avoid excluding important information which invalidates the results;
- *incomplete data sheets and insufficiently specified data*, indeed, in many cases, data is gathered from interviews and through question-

naires or from technical data sheets and database in which the information on the sought elements relates to other elements similar but not exactly equal to those studied, and often data are partially available.

Especially because of model uncertainties, it is become increasingly widespread, in many fields of engineering and sciences, accompanying practically all of the experimental data processing activities as well as many computational modeling and process simulation activities with *sensitivity analysis* [24]. The principle of a sensitivity analysis is simple: *change* the assumption, as that of some parameter definition, and *recalculate* the equations of the model to *confront* results. With this type of analysis it will get a better understanding of the magnitude of the effect of the assumptions made. It may find that the outcome of the recalculation can be quite heavily dependent on some of the assumed parameters.

3.1.3. Statistical approach to uncertainty

For a proper *uncertainty description* and statistical analysis of the variability of the observed quantities is essential to have good *visualizations* and *numerical synthesis* in order to allows to focus on important features of the data. Some characteristics of a dataset can be expressed numerically, for example, it is possible to characterize the position or central tendency of data by means of the usual *arithmetic average*. Since the dataset can be identified as a sample, this average is also called the *sample mean*. The latter is the average value of all observations in the dataset, x_i. These, in general, constitute a sample selected from a larger population of physical observations. It may therefore think of calculating the average value of all observations in a population so that sample mean is a reasonable estimate of the *population mean*, μ.

The variability or dispersion present in a sample of data may be described by the *sample variance* or the *sample standard deviation* (the positive square root of the sample variance). While the units of measurement of the mean and standard deviation are the same as the observed quantities, the unit of measurement of the variance is the square of that of the quantities. The sample variance is a *measure of the dispersion* because the bigger is the variability in the data, the greater are, in absolute value, some of the residues (differences between the value observed and the mean value). Since these, added together, always give zero-sum, it is necessary to use a measure of variability that transform the negative differences in positive amounts. Consequently, if the sample variance is little, the variability in the data is relatively low, and vice versa. Similar to the sample variance is the measure of variability in a population, the *population variance*, denoted by σ^2, is the square of the *population standard deviation* σ

$$\sigma^2 = \frac{\sum_{i=1}^{N}(x_i - \mu)^2}{N}$$

where N, is the size of the entire sample. In this way, Equation (3.1) can be rewritten as

$$\mu \pm \sigma$$

However, mean and variance are not the only indicators used to describe a data set. The *median* is a measure of the *center position* that divides the data into two equal parts, half below the median and half above; if the observations are equal in number, the median is halfway between the two middle values.

The *range* is a measure of the dispersion which can easily be calculated from the *difference between the maximum and minimum* of the dataset.

It is possible also to split data into several parts. When an ordered dataset is divided into four equal parts the points of division are called *quartiles*; the *first quartile* is a value that has approximately 25% of observations below and about 75% above it, the *second quartile* is exactly equal to the median and the *third* has about 75% of the observations below it. In general, the kth *percentile* (with k between 0 and 100) is the value such that a percentage equal to about k% of the observations are located at or below it, while about (100-k)% falls above.

As regards the *graphic representation* of the dispersion, besides the diagrams branches and leaves or the histograms, it is possible to use the *box plots*.

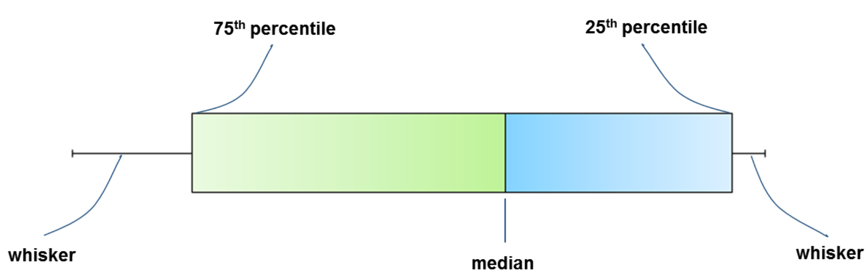


Figure 3.1 – Box plot description

Such a representation describes simultaneously the most important features of the data sets, such as the *center*, the dispersion, the *deviation from symmetry* and the identification of observations that fall unusually far from the main group of data, the so-called *outliers*. A box plot (Figure 3.1) represents the *three quartiles* aligned on a rectangular box. The box encloses the entire difference between the third and the first quartile with the lower side in correspondence of the 25th percentile and the upper of the 75th one. The middle line of the box is then drawn at the median. Outside of the opposite sides of the box stretch the *whiskers*; the lower one goes from the first quartile to the smallest observation within 1.5 interquartile difference, from the first quartile, while the upper whiskers is from third quartile to the largest observation within 1.5 interquartile differences, from the third quartile.

A mathematical model of a physical system need not necessarily to be a perfect abstraction: incorporating uncontrollable variables or inaccurate information, changes in the outcome measures are expected. The variables derived from the observations, the measured value of which may change from time to time, are defined random or aleatory variables, X. The *probability* is a concept used to quantify the likelihood, or *possibility*, that *a measurement falls within a given set of values*. "The possibility that X, the cost of an asset, is between 5000 and 5200 € is equal to 95%" is a statement that quantifies the feeling about the possible costs of that particular asset. The probability of a result can be interpreted as the *degree of subjective confidence* in the fact that this result may appear. As the probability of a result is in terms of *relative frequency* (per unit of total observations), referring to the cost of the asset mentioned, the relative frequency of repeated observations that fall in the range will be equal to 0.95. It can be written as

$$P\left(5000 \leq X \leq 5200\right) = 0.95$$

Not always an experiment produces a measured value and the values used in the models are not always derived from experimental observations. Sometimes a value can only be classified into a number of possible categories. Well, the concept of probability is applied in these cases too, and the interpretation in terms of frequency is still adequate [1].

The densities are commonly used in engineering to describe physical systems, similarly, a *probability density function* can be used to describe the probability distribution of a continuous random variable. The probability that X falls between a and b is then determined as the integral of $f(x)$ from a to b. The *probability density function of a continuous random variable* is used to determine the probability in the following way

$$P(a \le X \le b) = \int_a^b f(x)\,dx$$

The probability density functions are characterized by *positive functions*, the *probability can vary from 0 to 1* if, respectively, the values cannot occur or are certain. The function is used to calculate an area that represents the probability that the variable takes a value in the specified range. Furthermore, it is possible to synthesize the probability distribution by its mean and its variance.

The most widely used model for the distribution of a random variable is undoubtedly the *normal distribution*. It is also said *Gaussian* and has a symmetrical bell shape; each time a random experiment is repeated, the random variable, that is equal to the average result or total of replicas, tends to assume a normal distribution with increasing the number of replicates. The expected value of the distribution determines the center of the probability density function, that of variance determines its width. A random variable with probability density function

$$f(x) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

has a normal distribution and is said *normal random variable* with parameters μ e σ, the distribution is often indicated by the notation $N(\mu, \sigma^2)$. Since the probability density function decreases when moving away from the average, the probability that a measurement falls far from the expected value is low and from a certain distance, respect to the average, onwards can be approximated to zero. The area under the graph of a normal distribution over a certain distance equal to 3σ from the average is very small; since more than 99.73% of the probability of a normal distribution is within the range $(\mu \pm 3\sigma)$ as the width of the distribution is often indicated the value 6σ.

The variables of a system sometimes follow an exponential relationship as $x = e^w$. Whether the exponent is a random variable, W, then X is also a random variable. When W has a normal distribution then the distribution of X is said *lognormal* due to the calculation of the natural logarithm of X which therefore also appears to have a normal distribution. When W has mean θ and variance ω^2, $X = e^W$ is a *lognormal random variable* with probability density function

$$f\left(x\right)=\frac{1}{x\,\omega\sqrt{2\pi}}\,e^{\frac{-\left(\ln(x)-\theta\right)^2}{2\omega^2}}$$

The parameters of a lognormal distribution are θ and ω^2 but these are just the mean and variance of the random variable W. The lifetime of a product that will degrade over time is often modeled as a lognormal random variable.

There are also many other studied distributions, however, for the purposes of this thesis it may be more useful to turn an eye to simple distributions such as the range or the triangular one. The range, also known as *uniform distribution*, can simply be described by two variables: the *minimum* and the *maximum* values. This distribution is used when there is an equal probability that a quantity lies between a minimum and a maximum value [6].

When *a value* within the range has a *higher probability* to be observed the *triangular distribution* must be used. The latter is sometimes used as an alternative for the normal distribution, the advantage is that extremely high or low values cannot occur. As it is not said that the most probable value lies exactly in the middle of the range, this distribution can be used to approximate asymmetrical distributions as well as the lognormal one.

Statistical uncertainty and sensitivity analysis aim at assessing the contributions of the parameters uncertainties in contributing to the *overall uncertainty of the model output* [24]. Sampling-based analysis is performed in order to ascertain if model predictions fall within some region of concern and to identify the dominant parameters in contributing to the response uncertainty. The very first step of sampling-based analysis, in which uncertainties are assigned, is crucial to the results produced by the subsequent steps in the analysis because the results depend entirely on the *distributions assigned* to the sampled parameters, hence, the proper assignment of these distributions is essential to avoid producing bogus results.

3.2. Processing data and model uncertainties

All types of uncertainty affect directly or indirectly (through the model) the input data and propagate up to the results, the model outputs. The *uncertainty* of the *data* can be treated by defining a disturbance, a *perturbation* that affect the average or nominal data. The propagation of uncertainty to the results can be studied by applying the *Monte Carlo method*. Especially in the case of an Input-Output analysis, the Monte Carlo method is suggested to treat the propagation of uncertainty amongst the mathematical structures, such as matrixes and vectors, used. Lenzen [7] suggests that to assess the *propagation of uncertainty* in studies involving the Leontief inverse, the use of a Monte Carlo technique is necessary because it is not possible to carry out an analytical approach.

Besides, even using a *sensitivity analysis* of some assumptions globally, the changes performed on the input data, which continue to present some variability, propagate in final results. So, once again the best solution for the analysis is that to combine Monte Carlo method for data uncertainties with sensitivities analysis for model uncertainties [6]. Descriptive statistics then may be useful to summarize and show more effectively the analyses results.

3.2.1. Perturbation theory

The theory on the influence of *perturbation* of coefficients of matrixes on solutions of system of equations, can be used in *Input-Output analysis*. The quantities that describe the processes in Input-Output tables and so the coefficients that define the technology matrix often suffer from *uncertainty*. A statistical treatment of the *propagation* of these uncertainties is important even to investigate options for products improvement as such uncertainties affect ultimately *results*. However, the direct applicability of such approach is limited because the matrixes encountered in Input-Output analysis have particular characteristics, e.g. such matrixes are in most cases positive defined. Perturbation theory studies the influence of perturbations of equations coefficients on the solutions to those equations [25]. For example, by considering *Leontief's production model* expressed by Equation (3.2)

$$\boldsymbol{y} = \left(\boldsymbol{I} - \boldsymbol{A}\right)\boldsymbol{x} \tag{3.2}$$

a typical question addressed in perturbation theory is, given the above system, what would the solution be when the matrix $(\boldsymbol{I} - \boldsymbol{A})$, which for straightforwardness of writing can be simply called $\underline{\boldsymbol{A}}$, is perturbed, $\underline{\tilde{\boldsymbol{A}}}$

$$\left(\boldsymbol{I} - \tilde{\boldsymbol{A}}\right) = \underline{\tilde{\boldsymbol{A}}}$$

The Leontief's matrix inversion on the perturbed matrix can be used to find the new solution recalculating it, but can be also interesting to study how the perturbation propagates in the system. For this, we will consider the perturbed matrix to consist of the original matrix plus a *perturbation term*

$$\tilde{\underline{\boldsymbol{A}}} = \underline{\boldsymbol{A}} + \delta \underline{\boldsymbol{A}}$$

trying to derive expression for the solution perturbation term $\delta \boldsymbol{x}$, defined as

$$\tilde{\boldsymbol{x}} = \boldsymbol{x} + \delta \boldsymbol{x}$$

It is possible to study the effects of such a change in technology matrix on the result vector $\boldsymbol{x}$ starting from

$$\boldsymbol{y} = \left(\underline{\boldsymbol{A}} + \delta \underline{\boldsymbol{A}}\right)\left(\boldsymbol{x} + \delta \boldsymbol{x}\right)$$

Expanding the terms in parentheses

$$\boldsymbol{y} = \underline{\boldsymbol{A}}\,\boldsymbol{x} + \underline{\boldsymbol{A}}\,\delta \boldsymbol{x} + \delta \underline{\boldsymbol{A}}\,\boldsymbol{x} + \delta \underline{\boldsymbol{A}}\,\delta \boldsymbol{x}$$

As $\underline{\boldsymbol{A}}\,\boldsymbol{x} = \boldsymbol{y}$

$$\underline{\boldsymbol{A}}\,\delta \boldsymbol{x} + \delta \underline{\boldsymbol{A}}\,\boldsymbol{x} + \delta \underline{\boldsymbol{A}}\,\delta \boldsymbol{x} = 0$$

Assuming that $\tilde{\underline{\boldsymbol{A}}}$ is *invertible*

$$\delta \boldsymbol{x} = -(\underline{\boldsymbol{A}} + \delta \underline{\boldsymbol{A}})^{-1}\,\delta \underline{\boldsymbol{A}}\,\underline{\boldsymbol{A}}^{-1}\,\boldsymbol{y}$$

This important relationship enables to explore the study of perturbation theory and statistical analysis of the Input-Output analysis. Under the hypothesis of $\delta \underline{\boldsymbol{A}}$ infinitesimally small, $\underline{\boldsymbol{A}} + \delta \underline{\boldsymbol{A}} \cong \underline{\boldsymbol{A}}$, so

$$\frac{\partial \boldsymbol{x}}{\partial \underline{a}_{ij}} = -\underline{\boldsymbol{A}}^{-1}\,\frac{\partial \underline{\boldsymbol{A}}}{\partial \underline{a}_{ij}}\,\underline{\boldsymbol{A}}^{-1}\,\boldsymbol{y} \tag{3.3}$$

In agreement with the *differentiation rule* for inverse matrixes (e.g. Balestra [26]), it results

$$\frac{\partial \underline{\boldsymbol{A}}^{-1}}{\partial \underline{a}_{ij}} = -\underline{\boldsymbol{A}}^{-1}\,\frac{\partial \underline{\boldsymbol{A}}}{\partial \underline{a}_{ij}}\,\underline{\boldsymbol{A}}^{-1}$$

This way Equation (3.3) becomes

$$\frac{\partial \boldsymbol{x}}{\partial \underline{a}_{ij}} = \frac{\partial \underline{\boldsymbol{A}}^{-1}}{\partial \underline{a}_{ij}} \boldsymbol{y} + \underline{\boldsymbol{A}}^{-1} \frac{\partial \boldsymbol{y}}{\partial \underline{a}_{ij}} = \frac{\partial \underline{\boldsymbol{A}}^{-1}}{\partial \underline{a}_{ij}} \boldsymbol{y}$$

Thus, each coefficient of the vector $\partial \boldsymbol{x}/\partial \underline{\mathrm{a}}_{ij}$ depends on the individual elements of $\partial \underline{\boldsymbol{A}}^{-1}/\partial \underline{\mathrm{a}}_{ij}$. The knowledge of these derivatives opens the way to explore sensitivity and uncertainty analysis of all the derivatives $\partial x_k/\partial \underline{\mathrm{a}}_{ij}$ for each value of i and j.

Another important concept of matrix perturbation theory is the *condition number*. By considering perturbations in vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, the inequality for multiplications of *norms* yields

$$\|\delta \boldsymbol{x}\| \le \|\underline{\boldsymbol{A}}^{-1}\| \|\delta \boldsymbol{y}\|$$

But also

$$\|\boldsymbol{y}\| \le \|\underline{\boldsymbol{A}}\| \|\boldsymbol{x}\|$$

Thus, by combining these two equations

$$\frac{\|\delta \boldsymbol{x}\|}{\|\boldsymbol{x}\|} \le \|\underline{\boldsymbol{A}}\| \|\underline{\boldsymbol{A}}^{-1}\| \frac{\|\delta \boldsymbol{y}\|}{\|\boldsymbol{y}\|}$$

it is possible to measure how a relative change in $\boldsymbol{y}$ propagates as a relative change in $\boldsymbol{x}$. The factor

$$\kappa(\underline{\boldsymbol{A}}) = \|\underline{\boldsymbol{A}}\| \|\underline{\boldsymbol{A}}^{-1}\|$$

is known as the condition number of the matrix $\underline{\boldsymbol{A}}$; whenever such a number is large, relative variation in the vector of results may be very higher than in $\boldsymbol{y}$ and the solution of this kind of equations may be perturbed. A practical rule states that whenever the magnitude of a condition number is like 10^d then, in the solution of the equation, one can obtain $t - d$ correct digits, where t represents the correct digits of input values. For instance, when the input data is correct to 3 decimal places, a condition number of 100 means that 2 decimal point are lost in the solution to a system of equations, so that the solution is correct to 1 decimal place only. So, when data are quite imprecise to only 1 or 2 decimal places, a technology matrix with a condition number of 10 or 100 would deprive the result from any certainty: uncertainties in data and their propagation in the computations is therefore of theoretical and practical interest.

Perturbations in thermoeconomic Input-Output analysis because of uncertainties, can occur in the construction of the *exergetic table*, for example considering that fuel flows may not have constant exergy because of the variability of the different consignments of fuel used in the system, while being of the same type. So a perturbation will be produced also in vector of *final demand*. Moreover, uncertainty can be in *exogenous resources vector* since, for example, different enterprises can produce resources with similar but different costs. In any case, the perturbation can be studied as shown.

By considering a single unit process described by a *process vector* as

$$\boldsymbol{p} = \begin{pmatrix} p_1 \\ p_2 \\ \dots \end{pmatrix}$$

it is necessary to abandon the idea of point estimates, and include the idea that a distribution of values for the elements of this process vector exists. For simplicity, one can assume that this *distribution* is *Gaussian*. This enables to describe the distribution with mean μ and standard deviation σ. It is quite normal to write such a stochastic variable as $\mu \pm \sigma$, although this notation is sometimes used to indicate the range of possible values that the variable may attain. This way the process vector is

$$\tilde{\boldsymbol{p}} = \boldsymbol{p} + \delta \boldsymbol{p} = \begin{pmatrix} N(\mu_1, \sigma_1) \\ N(\mu_2, \sigma_2) \\ \dots \end{pmatrix}$$

In principle, every process vector may be defined this way and a stochastic process matrix may be constructed.

This is a conservative procedure, as it is based on the idea that all *uncertainties* are *independent* but in practice, this is not true: just think of the uncertainties on the exergy of a input as a fuel and the consequent uncertainties in the exergy of the exhausted gases. At any rate, it is likely that not all uncertainties are independent. In general, the degree of dependence between two random variables is measured by their covariance, the covariance between a variable and itself being the variance

$$\sigma_1^2 = \mathrm{cov}(\tilde{p}_1, \tilde{p}_1)$$

All the variances and covariances may be arranged in a matrix, the covariance matrix or dispersion matrix that is a symmetric matrix. The disadvantages of using this construction are: the reduction of information due to this symmetry, the fact that a very large matrix is necessary to represent all variances and covariances. In practice, covariances are almost never available in an empirical form. Only theoretical considerations, for example, on the basis of mass balances and chemical reaction theory can provide estimates of covariances.

Describing data *uncertainties* is like describing data to a certain sense; next step, is describing how to combine the variability in data into an overall uncertainty. For the combination of uncertainties there are other trends in addition to the distribution theory, as the categorical data quality description or the fuzzy set theory, but they are less used and there is not lot of literature available about them. Hence, the main approaches are that based on parametric variation, on analytical expression for error propagation or on *random experiments* for uncertainty propagation as those that adopt Monte Carlo techniques.

3.2.2. Monte Carlo technique

Monte Carlo analysis is a *sampling technique based on numerical simulation* in which a sample of engineering model results is generated and statistical properties of this sample are used to provide an indication of the *location* and *dispersion* of the *results* [27]. While analytical method are exact, sampling techniques provide stochastic results that are not exactly reproducible. However it should be noted that with analytical methods, approximations are often needed and that several authors [7] point out that, for particular models, such as those Input-Output, it is necessary to use random experiments for uncertainty propagation. Sampling techniques are able to deal with more than only a few theoretical distributions and can *include all* type of complicated *dependencies*. Especially when fast computers are available, Monte Carlo techniques provide a useful means of assessing robustness. Thermoeconomic Input-Output analysis is an area where it may be applied fruitfully. Having specified *probability distributions* for process data, one can proceed to generate one model realization. This yields a vector of results e.g. $\boldsymbol{c}$, that can be denote as $\boldsymbol{c}_1$. A second realization yields a second result $\boldsymbol{c}_2$, all together, after *model realizations*, a set of results $\{\boldsymbol{c}_1, \boldsymbol{c}_2, \dots, \boldsymbol{c}_N\}$ will be obtained and this set of results can be subject to analyses. In performing a Monte Carlo analysis, one must choose the *number of runs* N. It is important to underline that the number of uncertain input parameters does not affect the number of runs required. The latter is only determined by the required *accuracy of the output distribution* and the *computing capabilities available*.

After Monte Carlo development in the first half of the twentieth century, the method was continually in use and became a prominent instrument in the development of many projects and soon, applications started popping up in all sorts of situations in business, engineering, science and finance [28]. It is clear, then, that one of the main aspects of the method is to have available a reliable *random number generator*. This is a computerized or physical method that produces numbers that have *no sequential pattern* and are *arranged* purely *by chance*. Many computer languages have been developed to allow, in one way or another, to write codes for countless applications; languages as Visual Basic were popular in developing computer simulation models. The number of simulation software packages has also exploded over the years. Software include mathematical equations and algorithms associated with a given process. When the software fits the process under study, the user can apply it and quickly observe the outcomes from a new or modified arrangement of the process. This ability is a large *saving* in *time* and *cost of development*.

The models highly depend on the authenticity of the *algorithms* and on the choice of the input *probability distributions* and parameter values. An error in the formulation could give misleading results. Generating random numbers with use of a computer is not easy. One of the first tools used to generate random numbers is by way of the mathematical function called *modular arithmetic*. For a variable w, the modulo of w, modulus m, is denoted as $w\ modulo(m)$. The function modulo returns the remainder of w when divided by m. When w and m are integers, the function returns the remainder that also is an integer. Such a method and its advancements are one of the most common technique in use.

A series of *tests* have been developed in order to evaluate how good a sequence of uniform random variables are with respect to truly random uniform variables. The first consideration is how many random variables are generated before the cycle repeats. When the generated random numbers are set in intervals, the frequency for every interval of the numbers and the expected number of generated random numbers in an interval may be evaluated. With these two parameters a *Chi Square* (goodness-of-fit) *test* is used to determine if the sequence of generated numbers is spread equally in the considered range. Another test computes the *autocorrelation* between the generated random variables, the ideal is for all the autocorrelations to be significantly close to zero. These numbers are thereby called *pseudo random numbers* as they pretend to be random.

Whit the matrixes arrangement of an Input-Output analysis, the Monte Carlo method is suggested to treat the propagation of uncertainty. Lenzen [7], believing necessary the use of a Monte Carlo technique, stated that uncertainties in matrixes, as that of the technical coefficient $\boldsymbol{A}$, can be simulated by generating a matrix, $\delta\boldsymbol{A}$, which contains random perturbation. Moreover, Lenzen suggests that according to Quandt [29] it is possible to assume a normal distribution of uncertainty, even if Hanssen and Asbjørnsen [30] showed in their studies, that this is not always true. Moreover Kop Jansen [31] pointed out, because of the way Input-Output tables are constructed, uncertainties are correlated but the nature of this correlation and distribution is usually not known.

3.2.3. Uncertainty analysis, some numerical example

Before proceeding with the description of the used methodology for uncertainty evaluation in thermoeconomic Input-Output analysis, two *numerical example* of perturbation theory are provided simply to see how perturbation and uncertainty affect Leontief's production and cost models.

First, the uncertainty may affects the elements of the Input-Output table up to the technical coefficient matrix $\boldsymbol{A}$. For example, by considering *Leontief's production model*

$$\underline{\boldsymbol{A}}^{-1}\,\boldsymbol{y} = \boldsymbol{x}$$

$$\begin{pmatrix} 1.0050 & 0.9870 \\ 0.0019 & 1.0856 \end{pmatrix} \begin{pmatrix} 13.15 \\ 12.56 \end{pmatrix} = \begin{pmatrix} 25.61 \\ 13.66 \end{pmatrix}$$

the Leontief's inverse comes from the Input-Output matrix

$$\boldsymbol{E} = \begin{pmatrix} 0.0835 & 12.3789 \\ 0.0447 & 1.0554 \end{pmatrix}$$

in accordance with the theory presented in Chapter 2. When a *perturbation* is introduced as

$$\delta \boldsymbol{E} = \begin{pmatrix} 0 & -10 \\ 0 & 0 \end{pmatrix}$$

such that

$$\tilde{\boldsymbol{E}} = \boldsymbol{E} + \delta \boldsymbol{E}$$

$$\begin{pmatrix} 0.0835 & 2.3789 \\ 0.0447 & 1.0554 \end{pmatrix} = \begin{pmatrix} 0.0835 & 12.3789 \\ 0.0447 & 1.0554 \end{pmatrix} + \begin{pmatrix} 0 & -10 \\ 0 & 0 \end{pmatrix}$$

it propagates through Equation (2.15) up to the *Leontief's inverse* in such a way as to cause that it can be expressed as

$$\tilde{\underline{\boldsymbol{A}}}^{-1} = \underline{\boldsymbol{A}}^{-1} + \delta \underline{\boldsymbol{A}}^{-1}$$

$$\begin{pmatrix} 1.0036 & 0.1894 \\ 0.0019 & 1.0841 \end{pmatrix} = \begin{pmatrix} 1.0050 & 0.9870 \\ 0.0019 & 1.0856 \end{pmatrix} + \begin{pmatrix} -0.0014 & -0.7976 \\ 0.0000 & -0.0015 \end{pmatrix}$$

The condition number of the inverse is very low and equal to 3 so that the problem is not ill-conditioned. Hence, recalculating with the perturbed matrixes, the uncertainty reaches the *result vector* $\boldsymbol{x}$ as it is observable

$$\tilde{\boldsymbol{x}} = \boldsymbol{x} + \delta \boldsymbol{x}$$

$$\begin{pmatrix} 15.57 \\ 13.64 \end{pmatrix} = \begin{pmatrix} 25.61 \\ 13.66 \end{pmatrix} + \begin{pmatrix} -10.04 \\ -0.02 \end{pmatrix}$$

Next, for example in the *Leontief's cost model*, the uncertainty may affect the *exogenous resources vector*

$$\tilde{\boldsymbol{v}} = \boldsymbol{v} + \delta \boldsymbol{v}$$

$$\begin{pmatrix} 35.11 \\ 22.17 \end{pmatrix} = \begin{pmatrix} 30.11 \\ 13.17 \end{pmatrix} + \begin{pmatrix} 5 \\ 9 \end{pmatrix}$$

Since the specific cost are given, in accordance with Equation (2.14), by

$$\boldsymbol{c} = \left(\underline{\boldsymbol{A}}^{-1}\right)^T \boldsymbol{b}$$

$$\begin{pmatrix} 1.18 \\ 2.21 \end{pmatrix} = \begin{pmatrix} 1.0050 & 0.0019 \\ 0.9870 & 1.0856 \end{pmatrix} \begin{pmatrix} 1.18 \\ 0.96 \end{pmatrix}$$

in which the *specific exogenous resources vector* $\boldsymbol{b}$ is defined via Equation (2.12), it is possible to evaluate the propagation of uncertainty through the vector $\boldsymbol{b}$

$$\tilde{\boldsymbol{b}} = \boldsymbol{b} + \delta\boldsymbol{b}$$

$$\begin{pmatrix} 1.38 \\ 1.62 \end{pmatrix} = \begin{pmatrix} 1.18 \\ 0.96 \end{pmatrix} + \begin{pmatrix} 0.20 \\ 0.66 \end{pmatrix}$$

up to the result, the *cost vector*

$$\tilde{\boldsymbol{c}} = \boldsymbol{c} + \delta\boldsymbol{c}$$

$$\begin{pmatrix} 1.38 \\ 3.12 \end{pmatrix} = \begin{pmatrix} 1.18 \\ 2.21 \end{pmatrix} + \begin{pmatrix} 0.20 \\ 0.91 \end{pmatrix}$$

in which the perturbation is very different from that introduced as $\delta\mathbf{v}$. Furthermore, it should be mentioned that the uncertainties can affect the coefficients matrix and the resources vector at the same time with a propagation of effects due to different causes. Also because very rarely a change of value in a matrix or in a vector of the thermoeconomic Input-Output arrangement is not correlated with other changes and a perturbation produces other perturbations in cascade even before the application of the equations of the Leontief's models.

3.3. A method for uncertainty evaluation in thermoeconomic Input-Output analysis

In this thesis the methodology used for the evaluation of the uncertainty in thermoeconomic Input-Output analysis is the *Monte Carlo technique* for three main reasons:

1. to *handle uncertainty not only infinitesimally small*, the application of random experiments for uncertainty propagation is not subject to the limitations of the assumptions of the analytical approach;
2. to *estimate the correlations and the dependencies amongst the matrixes arrangement*, as it is not true that uncertainties are independent;
3. as indicated by the specific scientific *literature*, the studies by Lenzen [7] and Bullard and Sebald [32] among others.

Bearing in mind the discussion set forth in Chapter 2 and in Subparagraph 3.2.3, the uncertainty can be considered proper to the values that form the Input-Output table or can affect the values that make up the exogenous resources vector. A variation of the values of exergy input to the system, for example due to the *variability of the goods* for which the plant is supplied as raw materials for its operation, is reflected on a variability that accompanies the outputs produced by the system; and so is, even if the uncertainty is own of the exergetic vector of external resources. Some uncertainties can be also typical of the values of the *cost of the equipment* composing the system; this is true in the design phase when comparing the different possibilities offered by the market and not, of course, when studying a system that is already built, whit all costs known. But it is not always said that all the information required for the construction of this economic vector, even for an existing plant, can be known with certainty according to the resources available to the analyst. Furthermore, the degree of belief on the correctness of some information from assumptions on the model or the change in the definition of certain parameters of the model will result in uncertainties in the values of the results of the analysis.

Anyway, the variability can be represented thanks to the *perturbation theory*: each vector affected by uncertainty may be expressed as for the exogenous resources vector by

$$\tilde{\boldsymbol{v}} = \boldsymbol{v} + \delta\boldsymbol{v}$$

in which the perturbation $\delta\mathbf{v}$ may vary for every iteration of the *N Monte Carlo runs*. The number of *iterations* may be chosen based on the typical values found in the scientific literature, for example Bullard and Sebald [32] [33] suggest that 1000 iterations would be sufficient, to mediate between the resources spent to produce them and the quality of the results obtained. Hence, 1000 runs are adopted

$$\tilde{\boldsymbol{v}}_1 = \boldsymbol{v} + \delta\boldsymbol{v}_1 \qquad \tilde{\boldsymbol{v}}_2 = \boldsymbol{v} + \delta\boldsymbol{v}_2 \qquad \cdots \qquad \tilde{\boldsymbol{v}}_{1000} = \boldsymbol{v} + \delta\boldsymbol{v}_{1000}$$

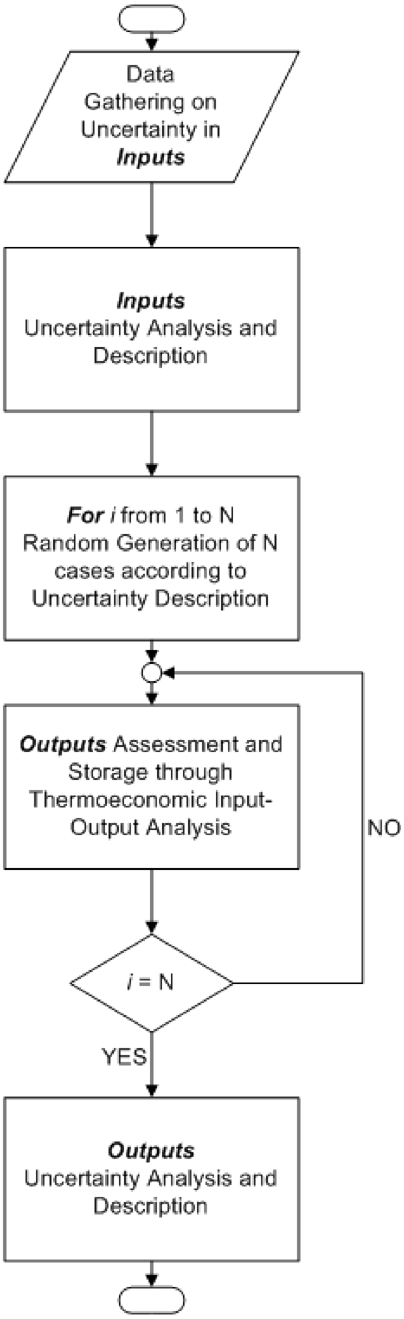
From each iteration the results of the thermoeconomic Input-Output analysis are, then, derived also characterized by variability

$$\left\{ \boldsymbol{c} + \delta \boldsymbol{c}_1, \boldsymbol{c} + \delta \boldsymbol{c}_2, \cdots, \boldsymbol{c} + \delta \boldsymbol{c}_{1000} \right\}$$

The variability can be introduced using known information about the data. When one knows the range of variation of a parameter, for which each value within the interval is equally probable, the quantity can be expressed through a *uniform distribution*, the range. In Excel this can be done by the function RANDBETWEEN. Consequently also the results, arising from inputs distributed this way, will have an almost uniform distribution. The inclusion of the values of the output when all the input ranges are at the *maximum* and *minimum value* in this type of analysis is essential because it provides information that is not said that the random analysis can consider. However it is not possible to do without the random analysis by a Monte Carlo technique because it simulates the propagation of more than one uncertainty up to results. A final definition of the interval as the output resulting from the minimum and maximum values of the input, it would not take into account a multiple propagation. Think of the definition of the thermodynamic variable f, the uncertainty of the exergoeconomic factor will result derived from uncertainty in investment costs plus that of the cost of the exergy destruction; with Monte Carlo simulations one does not risk to underestimate the range of variation of this result.

When it is possible to assume that the data distribution is normal, then the uncertainty in data may be described by the mean and the variance; in Excel the function NORMINV may be used together with the RAND function to simulate the probability and the results will be distributed according to the *Gaussian distribution*, evidently.

At each iteration, the output of the thermoeconomic Input-Output analysis, in Excel [34], can be *stored* by typing the command in Visual Basic to have, at the end of the simulations, all the results in order to proceed with their *analysis*. In addition to the graphic presentation by means of box plots, output may be described through drawing intervals with the representation of the quartiles in which the values of the studied results are included. In Figure 3.2 a schematic representation of the passages for the application of the method is presented.



Inputs: elements of Input-Output matrix or exogenous resources vector
Outputs: costs and specific costs of product and fuel & thermoeconomic variables

Figure 3.2 – Monte Carlo method for Input-Output analysis diagram

4. Casalvolone Anaerobic Digester

The analyzed *case study* is an existing plant of anaerobic bio-digestion. This plant is taken as an *example* to show the application of the method of uncertainty evaluation in an thermoeconomic Input-Output analysis.

4.1. Introduction to anaerobic digestion

A biomass classification may be done on the quantity of water possessed: if the amount of water is lower than 50%, biomass will be classified as relatively dry; if the amount of water is greater than 80%, biomass will be categorized as definitely moist; if the water is present in a percentage between 50 e 80%, it will be possible to decide whether to dilute the biomass in order to continue the treatment with a wet processing or to dry the biomass in order to use it as a fuel. Depending on the type of *biomass*, on the investable capital and on the presence or absence of incentives it should be identified the optimal process (dry or wet) for the production of energy. This process consist in the transformation of the chemical energy owned by the biomass in another form of available energy: thermal and/or electric energy. Transformations can lead to formation of not properly energetic byproducts (e.g. glycerol for the production process of biodiesel or digestate for the production process of biogas).

Besides the thermochemical (combustion, gasification, pyrolysis) and chemical (e.g. transesterification) processes, biologic processes, as the anaerobic digestion and the fermentation may convert the form of energy contained in the biomass in heat and work. If the water content in the biomass is high, when the energy consumption to dry the biomass is not justified or if the plant cost for the drying process becomes too high, the biochemical *conversion* represents the best way to exploit the energy content of the biomass and the anaerobic digestion is normally the adopted process.

4.1.1. Biomass digestion

The use of different types of dedicated and waste biomass has led to the development of various types of *anaerobic digestion* processes and different technologies, mainly based on the dry matter content of the substrate fed into the reactor [35]. Therefore, based on the *total solids content*, there are three different techniques:

1. *wet digestion*, when the substrate in the digestion has a dry substance content below 10%, this is the most common technique, particularly with animal slurry;
2. *semi-dry digestion*, with intermediate values of dry matter, 10-20%, this process is less common;
3. *dry digestion*, when the substrate in the digestion has dry substance content exceeding 20%.

The choice to work in separate or individual phases is subject to the characteristics of the substrate: highly biodegradable substrates are more difficult to manage with one-phase processes. The *anaerobic microorganisms* have low growth rate and low rate of reaction and therefore it is necessary to keep *optimum* the *conditions* of the reaction environment. The latter, usually defined *anaerobic reactor*, to allow the simultaneous growth of all the microorganisms involved, shall result from a compromise between the needs of individual microbial groups.

The rate of net increase of digestion on a given substrate is a function of the internal temperature of the digester and the type of bacteria and the rate of use of biomass which depends on the concentration and the affinity between bacteria and biomass. Increasing the *concentration of substrate*, it is possible to approach the maximum possible rate; other important parameters are *pH* (7-7.5 optimum value for the methanogenesis), *alkalinity* and the *production and percentage composition of the biogas*. The anaerobic biological activity is possible in a wide *temperature* range, between –5 and +70 °C with various microorganisms classified according to the optimal thermal interval of growth:

- *psychrophilic bacteria* (temperatures below 20 °C);
- *mesophilic bacteria* (temperatures between 20 °C and 40 °C);
- *thermophilic bacteria* (temperatures above 45 °C).

The activity of the bacteria, however, increases with temperature so that a higher temperature, becoming more rapid gas production, results in a lower *retention time* of the material inside the digester. On average, with mesophilic bacteria 16-30 days are necessary, while with thermophilic bacteria the range decreases to 14-16 days. The choice of temperature then comes from a compromise between gas production and possible maximum temperature, which must be such as not to destroy the enzymes; so insulations and systems for heating the biomass within the digester are used.

The *percentage of methane* in the produced biogas varies, depending on the type of digested biomass and on the conditions in the reactor, from a minimum of 50% to a maximum of 80%. The biomass subjected to anaerobic digestion is defined by a few parameters easy to measure like:

- the *total solids* or dry substance (% on wet basis) is the dry matter content, determined by drying at 105 °C and representing the sum of the organic substance and the inert substance;
- the *volatile matter* (% of dry matter) is the fraction of organic matter that can volatilize, about 80% of the total organic, operationally it is assumed that the volatile substance is equal to the organic matter.

The *biomass conversion* leads to degradation of the sugars, even of cellulose, through various reactions that produce a *biogas* consisting primarily of *methane* and *carbon dioxide* and *digestate* (the material remaining from biodegradable feedstock after the digestion that produce biogas). Schematically, four key biological and chemical stages happen:

1. *hydrolysis*, the complex organic molecules are broken into simple sugar, amino acids and fatty acids;
2. *acidogenesis*, there is further breakdown of remaining components into volatile fatty acids, ammonia, carbon dioxide and hydrogen sulfide;
3. *acetogenesis*, simple molecules are further digested to produce largely acetic acid, as well as carbon dioxide and hydrogen;
4. *methanogenesis*, bacteria digest the acids into methane, carbon dioxide and water.

For the success of the process of methanisation is important the retention time, or the *residence time*, defined as the residence time of the organic mass in the digester. The biogas production increases with the retention time: initially zero, within a few days reaches the maximum and then decreases slowly with a bell-shaped trend. The *hydraulic retention time* τ represents the residence time of each fluid element within the reactor or the average of the residence times in the reactor of the individual fluid elements.

$$\tau = \frac{V_{reactor}}{\dot{V}_{F,IN}} \qquad (4.1)$$

where $V_{reactor}$ is the volume of the reactor, $\dot{V}_{F,IN}$ is the volumetric flow rate of the total amount at the reactor inlet and the retention time is usually expressed in days.

Several biomasses, treatable anaerobically, have a *content of sulfur* compounds that is not negligible for the purposes of the digestion process. The main form of sulfur compounds is that of sulfate, which, in the environment of the strongly reducing anaerobic reactor, is soon converted into sulphide. The presence of sulfur compounds promotes the growth of sulfate reducing bacteria that compete with methanogenic bacteria in the use of acetic acid and hydrogen.

In wet processes the biomass is treated so as to have a *total solids content* less than 10% in order to be able to use a classic continuous agitated-tank reactor. The biomass, before being loaded into the anaerobic reactor, undergoes a treatment aimed at achieving a proper content of total solids and of a good level of homogenization; it consists mainly of a *dilution* carried out by addition of water (slurry and/or process water) and of a removal of any foam, plastics or other coarse materials which are potentially damaging to the mechanics of the plant. The reactor most frequently used in this type of process is the classic *continuous stirred-tank reactor* (CSTR).

4.1.2. Stages of a digestion plant

Firstly near the farm is realized a *storage site*, where the livestock manure, collected through a mechanical recovery manure system, and the vegetal biomass are stored and accumulated. It is important to avoid that in this site reactions which lead to the formation of methane can occur and so the detention time in the storage site must be as low as possible. Any methane production would be, in fact, very harmful, not only for the possible environmental pollution, but also because it would reduce the methane production in the digester itself, thus going to reduce also the overall efficiency.

Anaerobic digestion is a process of biological conversion, in oxygen absence, through which approximately 50% of the organic substance contained in the input matter is transformed into biogas consisting in methane, carbon dioxide and traces of water, nitrogen, hydrogen and pollutants. The *digester* can be single or double-stage, and can be characterized by a cold digestion or by a heated digestion. The choice is at the discretion of the designer and depends on the process parameters to optimize. To choose a configuration over another one availability of biomass, financial resources, infrastructure, space, sanitation requirements, climate (because a cold climate requires better insulation) and time of storage must be taken into account. Within the reactor, the substrate in the digestion phase should be properly mixed, so as to: facilitate contact between bacteria and substrate, avoid the presence of dead zones, ensure a homogeneous temperature distribution, optimize the release of biogas and prevent settling of the sludge and the formation of surface crusts. The *mechanical agitators* are generally subject to abrasion and clogging, due to the presence of hard or fibrous particles, and therefore they require frequent maintenance.

The *digestate* is collected and stored in *tanks*; it can be used as soil improver, downstream of a chemical-physical analysis aimed to detect within it the presence of possible contaminants to the soil. The positive outcome of the analysis allows the direct use of digestate as fertilizer in agriculture, otherwise it is necessary to establish a system of digestate treatment.

The operation of the equipment connected to the biogas must be continuous while the diagram of the production may be subject to temporal variations. It is therefore necessary to have a storage system with a volume able to equalize the fluctuations of production so as to not having to stop the machines of the plant or release the gas in the torch to prevent dispersion in the environment. The *gas storages*, also called gas holders, have variable volume and low pressure that can be variable or constant.

The *biogas*, after undergoing the *treatments* required to reduce the presence of moisture, sulfur compounds and particulates, is controlled and sent to *electrical power production*. The electricity generated in cogeneration is fed into the electricity grid via a parallel connection with the alternator. In the event the grid has a voltage different from that of the electricity produced, it is necessary to raise it by means of a transformer substation.

In the design of the anaerobic digestion units, it is also necessary to pay attention to the construction aspects related to the system of charging and discharging the mixture from the digester and to the handling of sludge. The loading/unloading system must be made in such a way that, introduction of air mass in the reactor and leaks of matter or of biogas from the reactor does not occur. The unloading system must allow the dosage of the digested material to the next stage of the process. It must be thus provided a control system which prevents accidental emptying of the digester during unloading. Irrespective of the loading/unloading system, the digester must be equipped with a protection system to the pressure and the vacuum.

4.2. Description of Casalvolone digester

The analyzed existing anaerobic digester is that in *Casalvolone* in the Province of Novara, Piedmont. This is one of the more than 500 agricultural biogas plants present nowadays in Italy [36]. Public incentives for electricity production and heat valorization from biogas are granted, so biogas is utilized to feed combined heat and power generation plant (CHP) engine. According to Fantozzi and Buratti [37] Casalvolone plant reactor can be analyzed as a *CSTR*. As in plants of other European countries the usage of cereal silage, regarding the feeding of reactor, is accompanied by digestion of *animal manure*, this represents one of the best technique for an *energy valorization* of this byproducts, moreover this lead to a reduction of methane emission during storage of manure.

4.2.1. Main features

Casalvolone plant has an *installed power* of 999 kW_{el} and co-digests *maize silage* and *pig slurry* respectively in percentage of 54.5 and 45.5%. The CHP engine of the plant has *electrical* and *thermal efficiencies* such that the 40.7% of the power available to the engine (as biogas heating value) is converted into electricity and the 44.0%, instead, is converted into heat available as hot water. Figure 4.1 shows the main components of the plant.

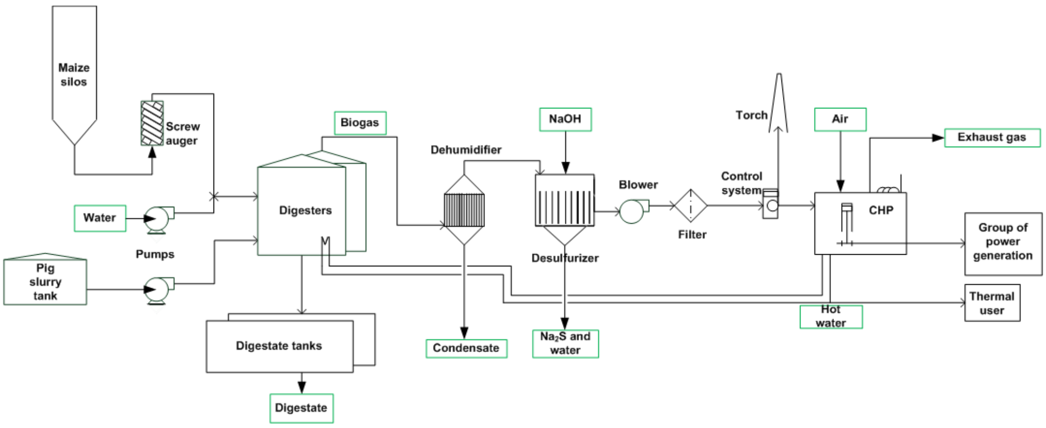


Figure 4.1 – Casalvolone plant diagram, main components

The maize is stored in *silos* at the biogas plant, where it is ensiled. This biomass is transported from the field to the biogas plant with farm tipping trailers. The transport of pig slurry is done by sludge tanks. During ensiling and storage operations, some biomass is lost, in fact, a *maize loss* of 2% is considered while for pig slurry no losses occur, considering that it is moved through pipelines. In the loading phase the solid biomass is fed into the digester through a *screw auger*, which requires 65 kW, placed on the bottom of a hopper in which the maize silage is loaded by tractor coupled with a frontal loader. *Pig slurry* is introduced in the digesters by means of a *pump* requiring 20 kW. The *water* utilized for *dilution* of feedstock is introduced using a *pump* requiring 15 kW; so within the reactor, dry matter content is about 10%.

Inside the two *digesters* the temperature is kept in mesophilic conditions to 40 °C by hot water coming from the engine jacket. Such a water is moved by 4 pumps, entailing 1.5 kW consumption, in the *heat exchangers* on the digester wall. Single-stage digestion takes place in continuous stirred-tank reactors. Furthermore, each digester has *submerged mixers* with an electrical power of 13 kW for homogenization of feedstock and liquid fraction and a pump for the digestate discharge requiring 22 kW. The biogas produced as a result of the digestion of organic matter is stored in the gasholder dome placed on the top of the digester.

The *biogas* that leaves the reactor is filtered in a sand filter, dehumidified and desulfurized. Dehumidification is due to a *refrigeration unit* of 15 kW which cools down the biogas temperature removing the water vapor while desulfurization is due to NaOH in a *wet scrubber* that requires 10 kW.

Energy conversion occurs in the CHP unit that runs constantly at 1500 rpm and where biogas is burnt in an internal combustion engine with an *electrical* power generation of 999 kW_{el} and a *thermal* one of 1100 kW_{th}. More precisely, the CHP recovers the heat from both the engine water cooling jackets (at about 70 °C) and the exhaust gases (at 150 °C). Maize silage and pig slurry properties have been studied experimentally by Fiala [38] and are reported in the following Table 4.1

Biomass	**Total solids** % of wet bases	**Volatile solids** % of total solids	**Produced biogas** $m^3_N/t_{volatile\ solids}$	**Methane in biogas** % volume
Pig slurry	3.5	85	450	60
Maize silage	38.0	90	650	53

Table 4.1 – Characteristics of biomass

Considering such characteristics, a *dilution* of the maize silage is required, it is carried out with water that can come from liquid fraction of digestate. One ton of feedstock mixture corresponds with about 0.9 t of digestate; the latter can partially be separated into solid and liquid fraction and it is spread in the fields as organic fertilizer. Every day in the digester are introduced 55 t of *maize silage*, 45 t of *pig slurry* end 120 t of *water for dilution* on wet basis and, always on a daily basis, are produced by the plant 203 t of *digestate*. According to Dressler et al. [39] *biogas losses* from digesters, biogas treatment devices and CHP can be estimated in the order of 1.5%. Methane losses can be quantified for this plant equal to 91.5 m^3_N/day on a total biogas production of 11438 m^3_N/day; the subscript N is referred to normal conditions of temperature and pressure at 273.15 K and 101325 Pa. In Table 4.2 *gross and net production and self-consumption of electricity and heat* may be observed

	Gross production	Self-consumption	Net production
Electricity (kWh_{el}/d)	23982	1758	22224
Heat (kWh_{th}/d)	25927	8303	17624

Table 4.2 – Electricity and heat production

Specific heat consumption per produced biogas is 0.726 kWh_{th}/m^3_N, while, per produced net electricity it is equal to 0.373 kWh_{th}/kWh_{el}.

4.3. Plant thermodynamic model

From information provided by the study of Bacenetti et al. [36] the *thermodynamic model* of the Casalvolone anaerobic digestion plant has been constructed. Here it is presented in stages of the conversion process: *load*, *digesters*, *biogas treatment* and *power production*. Then, the main and fundamental *exergy flows* have been evaluated.

4.3.1. Loading stage

The *mass flow rate* of the maize is 0.63 kg/s, that of slurry 0.53 kg/s with a flow rate of water equal to 1.39 kg/s. In Table 4.3 the *mass fractions* of the feedstocks are indicated.

Feedstock	y
Maize	0.25
Slurry	0.21
Water	0.54

Table 4.3 – Mass fractions of feedstocks

Hence, the *total flow rate* has been calculated by the sum *of the three feedstocks* to the value of 2.55 kg/s (220 t/d). Once familiar with the percentage of the dry solid fraction of the maize and the slurry, it can be concluded that 62% of maize and 97% of the slurry is made of *moisture*. By considering the aforementioned *maize loss* $\Delta\dot{m}_{maize,dry}$ through equation

$$\dot{m}_{maize,\mathrm{dry}} = \dot{m}_{maize}\,(1-\Delta\dot{m}_{maize})\,y_{maize,\mathrm{dry}}$$

a *mass flow rate of dry maize* of 0.23 kg/s (20.3 t/d) has been evaluated. Similarly *flow rate of dry slurry* is found to be equal to 0.02 kg/s (1.6 t/d) and that of *water plus the biomasses moistures* to 2.29 kg/s (197.7 t/d) via

$$\dot{m}_{water,\mathrm{tot}} = \dot{m}_{maize}\left(1 - y_{maize,\mathrm{dry}}\right) + \dot{m}_{slurry}\left(1 - y_{slurry,\mathrm{dry}}\right) + \dot{m}_{water}$$

Thus, as said, it has been possible to estimate the *dry mass fractions of the feedstocks*, as shown in Table 4.4,

Feedstock	y_{dry}
Maize	0.09
Slurry	0.01
Water	0.90

Table 4.4 – Dry mass fractions of feedstocks

in order to verify that only 10% of feedstock consists of *dry matter* capable of producing biogas.

The evaluation of the *heating value* of the biomasses deserves a separate discussion. The elemental *chemical composition of the maize* has been assumed from Fiala [38] and is presented, on *dry basis*, in Table 4.5. From such a composition, by knowing the percentage of dry fraction and by normalizing results, it has been possible to estimate the *mass fraction* of all chemical elements; moreover, inasmuch as

$$Mm = \frac{1}{\sum_i \frac{y_i}{Mm_i}} \quad ; \quad x_i = y_i \frac{Mm}{Mm_i}$$

with Mm, *molar mass of the maize* equal to 6.4 kg/kmol, also *mole fractions* x_i of all elements have been estimated and all the results are in Table 4.5.

Element	y_{dry}	y	x
C	0.429	0.163	0.087
H	0.073	0.097	0.618
O	0.481	0.733	0.294
N	0.002	0.001	0.000
S	0.001	0.000	0.000
Cl	0.002	0.001	0.000
Ash	0.012	0.005	0.000

Table 4.5 – Elemental composition of maize

Through a Dulong empirical relationship [40] the *higher heating value of the maize* has been so calculated

$$HHV = 32.79\, y_C + 150.4\left(y_H - \frac{y_O}{8} \right) + 9.26\, y_S + 4.97\, y_O + 2.42\, y_N \quad (4.2)$$

at the value of 9.8 MJ/kg as the empirical coefficient in Equation (4.2) are expressed in such units. As regards the slurry, instead, since there are no studies on its elemental composition, it has been necessary proceed with the *assumptions from the composition of the solid faeces*. These assumptions are justified by the fact that 97% of the pig slurry is composed of water, so they only affect a small percentage of the total composition of this feedstock. Faeces are mainly composed by fiber, bacteria, fat, protein, and substances that can be classified as ashes in percentages and compositions that can be deduced from scientific literature. For example, for the fatty acids, from stearic to oleic one, passing through all the different types, compositions in terms of carbon, oxygen and hydrogen are known, thus it has been possible to estimate the average mole compositions and so for all constituents of the faeces. The *elemental chemical composition* utilized in this thesis *for the pig slurry* is hence reported in Table 4.6. This way, to evaluate the *higher heating value of the slurry* Equation (4.2) has been applied to obtain 5.1 MJ/kg. Once evaluated biomasses HHVs the *power of feedstock mix into the reactors* has been calculated on the value of 4500 kW through the relation

$$\dot{Q}_{F,IN} = \dot{m}_{maize}\, y_{maize,\mathrm{dry}}\, LHV_{maize,\mathrm{dry}} + \dot{m}_{slurry}\, y_{slurry,\mathrm{dry}}\, LHV_{slurry,\mathrm{dry}}$$

where the *lower heating value of dry biomasses* have been estimated, by considering the dry mass compositions and the evaporation enthalpy of water, to the values of 17.0 MJ/kg_{dry} and 22.5 MJ/kg_{dry} respectively for the maize and the slurry.

Element	y_{dry}	y	x
C	0.421	0.015	0.007
H	0.073	0.111	0.663
O	0.320	0.868	0.328
N	0.017	0.001	0.000
Ash	0.170	0.006	0.001

Table 4.6 – Elemental composition of slurry

The *retention time* has been considered to be equal to 20 days in accordance with an article of Campi et al. [41]. The *volumetric flow rate of the feedstock mix* introduced into the reactor has been estimated to be equal to 261.6 m^3/d as the used *densities* are equal to 568 kg/m^3, 1000 kg/m^3 and 999 kg/m^3 respectively for the *maize*, the *slurry* and *water*. This way, through

Equation (4.1) the *volume of the reactor* has been calculated to 5231 m^3. Thanks to an interview to a technician of the EnviTec Biogas, the manufacturing company of the plant, it has been discovered that the reactors have a *standard form* of 25 m in diameter and 6 m in height. Thus it is clear that the total amount of the volume is considered be split into *2 reactors*.

4.3.2. Digestion stage

In the reactors, a fraction of biomass becomes biogas, such conversion has not been studied through a discussion centered on the set of chemical reactions that occur in the digester, but taking into consideration the *information* present on *the experimental production of methane from biomasses* by Fiala [38] shown in Table 4.1. In Table 4.7 is presented the *composition* (*mole fractions*) assumed and estimated *of the biogas*

Molecule	x_{maize}	x_{slurry}
CH_4	0.530	0.600
CO_2	0.413	0.343
H_2O	0.044	0.044
H_2S	0.003	0.000
H_2	0.001	0.004
N_2	0.010	0.010

Table 4.7 – Molecular composition of biogas by different biomasses

Where the fraction of the methane is known and that of the carbon dioxide is derived as a complement to one, since the CO_2 is the main component of biogas together with CH_4, while the fractions of water and hydrogen sulfide have been estimated from an article of Bacenetti and Negri [42]. The fraction of hydrogen has been assumed while the nitrogen one comes from a technical report of an anaerobic digester plant by Giommi [43]. The *total volumetric flow rate of biogas* has been calculated by multiplying the mass flow rates of biomasses by the percentages of volatile solid and by the conversion factors of produced biogas, all shown in Table 4.1 to get a value of 12482.2 m^3_N/d (0.14 m^3_N/s). To undertake an evaluation of the total composition of the biogas, the *flow rates of biogas from the maize and from the slurry* have been expressed *in mole terms* through

$$\dot{n}_{biogas} = \frac{\dot{V}_{biogas}\, p_N}{R\, T_N}$$

to obtain 529.7 kmol/d (0.0061 kmol/s) and 27.2 kmol/d (0.0003 kmol/s), respectively. In this way, it has been possible to evaluate the mole flow rates for each chemical species and for each biomass of the plant. Through the estimation of the *molar mass of the biogas in the digesters*

$$Mm = \sum_i x_i \; Mm_i$$

to the value of 27.7 kg/kmol, the *composition of biogas at the exit of the reactors* has been calculated and results are shown in Table 4.8.

Molecule	ṅ (kmol/s)	x	y	ṁ (kg/s)
CH_4	0.0034	0.53	0.31	0.0552
CO_2	0.0026	0.42	0.65	0.1161
H_2O	0.0003	0.04	0.03	0.0051
H_2S	0.0000	0.00	0.00	0.0006
H_2	0.0000	0.00	0.00	0.0000
N_2	0.0001	0.01	0.01	0.0018

Table 4.8 – Composition and flow rates of biogas at reactor exit

The *conditions in the reactor* are a temperature of 313.15 K [36] and a pressure of 500 Pa [43]. Since the saturation pressure of water at this temperature is equal to 7384 Pa, no vapor slip occur within the biogas, or rather, the flow rate of water within the biogas flow does not change. Thus, the *flow rate of biogas* can be expressed *in mole quantities* to 556.9 kmol/d (0.0064 kmol/s) or in *mass quantities* at 0.1787 kg/s (15.4 t/d) *at reactor exit*. From the digesters also the *digestate* comes out, simply as a difference coming from mass balance at the reactor

$$\dot{m}_{digestate} = \left(\dot{m}_{F,IN} - \dot{m}_{biogas} \right)_{reactor}$$

Its *mass flow rate* is equal to 204.6 t/d.

4.3.3. Biogas treatments stage

In accordance with Bacenetti and Negri's article [42] it is possible to derive the *removal efficiencies of water vapor and of sulfur from biogas*: efficiencies of 95% and 97%, respectively, have been assumed. The treatments in the *dehumidifier* and in the *desulfurizer* produce variations in the composition of the biogas, at the end of these processes, the composition is that observable in Table 4.9 with a molar mass of 28.1 kg/kmol.

Molecule	$\dot{n}$ (kmol/s)	x	y	$\dot{m}$ (kg/s)
CH_4	0.0034	0.56	0.32	0.0552
CO_2	0.0026	0.43	0.67	0.1161
H_2O	0.0000	0.00	0.00	0.0003
H_2S	0.0000	0.00	0.00	0.0000
H_2	0.0000	0.00	0.00	0.0000
N_2	0.0001	0.01	0.01	0.0018

Table 4.9 – Composition and flow rates of biogas at biogas treatments exit

Hence, *mole flow rate* at the end of treatments has been evaluated to the value of 0.0062 kmol/s and *mass flow rate* to the value of 0.1733 kg/s. In this stage, according to Bacenetti et al. [36] a 1% *biogas loss* has been considered. This has led to *a reduction of the flow rates* to the values of 527.0 kmol/d (0.0061 kmol/s, 11811.7 m^3_N/d) and 14.7 t/d (0.1716 kg/s). The *lower heating value of the treated biogas* has been calculated equal to 15.9 MJ/kg via

$$LHV = \sum_i y_i \, LHV_i$$

considering the mass composition of biogas and the LHV of each chemical species.

4.3.4. Power production stage

In accordance with another article by Bacenetti et al. [44] the *daily availability* of the CHP engine has been considered equal to 21.92 h. Also taking account of the abovementioned relative *loss* on the 0.5% in conversion of biogas *into the engine*, and of an absolute one regarding methane fraction, the actual *flow rates of fuel input to the CHP engine* have been evaluated: a *mole* flow rate of 471.5 kmol/d (0.0055 kmol/s) and a *mass* flow rate of 13.3 t/d (0.1535 kg/s). As the 41% of biogas power (LHV) is converted into electrical power and the 44% in thermal power, by multiplying mass flow rate by LHV of biogas for these two efficiencies, *gross electrical* and *thermal powers* have been estimated to the values of 995 kW and 1076 kW respectively. By considering all the *auxiliaries*, the power for the screw auger of maize, for the pumps of slurry, feed-water and hot water for the reactor, for agitators of reactor, for digestate handlings, for dehumidifier, for desulfurizer and for the blower of biogas, a *needed power* of 207 kW has been estimated, so, the *net power* produced by the plant can be evaluated to 789 kW. Taking account of a 32% *self-consumption of thermal power* [36] even the *net thermal power* produced by the digestion plant has been calculated to the value of

732 kW. Also the produced *energies* per time unit have been estimated by considering the obtained results, for a comparison with the data of the real plant, and a 7.5% *self-consumption of electricity* [36], the results are shown in Table 4.10

	Gross production	Self-consumption	Net production
Electricity (kWh_{el}/d)	23884	1791	22093
Heat (kWh_{th}/d)	25821	8263	17558

Table 4.10 – Calculated electricity and heat production

The *specific heat consumption* per produced biogas has been assessed to the value of 0.782 kWh_{th}/m^3_N and the specific heat consumption per produced net electricity to 0.374 kWh_{th}/kWh_{el}. Accordingly, the gotten *results*, starting from the actual data of the system and from the assumptions made in the model, *agree with the data gathered* in the existing plant.

Different efficiencies of Casalvolone plant have been evaluated. Regarding the *heating value of the biomasses*,

$$\eta_{el} = \frac{\dot{W}_{net}}{\dot{Q}_{F,IN}}$$

the *electrical efficiency* to 18%, considering the ratio between net electrical power of the plant and the power entering the system with the biomasses.

$$\eta_{th} = \frac{\dot{Q}_{net}}{\dot{Q}_{F,IN}}$$

The *thermal efficiency* to a value of 16%, considering the net thermal power.

$$\eta_{I} = \frac{\dot{W}_{net} + \dot{Q}_{net}}{\dot{Q}_{F,IN}}$$

The *first law efficiency* as sum of the first two.

$$\eta_{II} = \frac{\dot{W}_{net} + \dot{Q}_{net}\left(1 - \frac{T_0}{\bar{T}_{\ln,th}}\right)}{\dot{Q}_{F,IN}}$$

The *second law efficiency*, getting the value of 19%, takes into account the quality of the output produced by the plant by weighting the thermal power with Carnot factor. Where the *average temperature* of the flow has been evaluated at a temperature of 336.71 K using the expression

$$\bar{T}_{\ln,exc} = \frac{T_{IN,exc} - T_{OUT,exc}}{\ln \frac{T_{IN,exc}}{T_{OUT,exc}}}$$

as a thermal user inlet temperature of 85 °C and an output one of 43 °C have been assumed. Regarding the *heating value of the biogas*, instead, with analogous expressions have been calculated the values of 32%, 30%, 62% and 36% respectively for electrical, thermal, first and second law efficiency. Finally, the *index of energy saving*, IRE, has been estimated to the value of 12% through

$$IRE = 1 - \frac{\left(\dot{m}\, LHV\right)_{biogas,\mathrm{CHP}}}{\frac{\dot{W}_{net}}{\eta_{el,\mathrm{ref}}} + \frac{\dot{Q}_{net}}{\eta_{th,\mathrm{ref}}}}$$

where the *reference electrical*, $\eta_{el,ref}$, and *thermal efficiencies*, $\eta_{th,ref}$, to the values of 40% and 90%, have been derived from Italian electricity and gas Authority [45] [46].

4.3.5. Estimating exergy flows

For the evaluation of the exergy flows, a simplification on the conception of the plant structure, which leads to the analysis of the *main nine components*, has been performed, in a fuel and product logic. The nine components taken into consideration are: the screw auger, the water pump, the slurry pump, the digesters, the digestate tanks, the dehumidifier, the desulfurizer, the blower with the filter and the control system and, at last, the CHP engine. In each component, there are input and output exergy flows both linked to *materials flows* and to energy flows, but, among these, only those which constitute a useful output for the component and the system are taken into account; e.g. the flow of condensate exiting the dehumidifier or the flow of exhaust gases from CHP engine have not been considered. In Table 4.11 are shown the compositions and the conditions of the mass flows from which exergy flows have been estimated as exposed in Table 4.12.

	y_C	y_H	y_O	y_N	y_S	y_{Cl}	y_{Ash}	p (Pa)	T (°C)	ṁ (kg/s)
Maize IN plant	0.163	0.097	0.733	0.001	0.000	0.001	0.005	101325	25	0.631
Maize IN reactor	0.163	0.097	0.733	0.001	0.000	0.001	0.005	101325	25	0.618
Water IN plant	-	0.112	0.888	-	-	-	-	250000	15	1.389
Water IN reactor	-	0.112	0.888	-	-	-	-	1150000	25	1.389
Slurry IN plant	0.015	0.111	0.868	0.001	-	-	0.006	101325	25	0.527
Slurry IN reactor	0.015	0.111	0.868	0.001	-	-	0.006	601325	25	0.527
Biogas IN dehumidifier	0.408	0.081	0.497	0.010	0.003	-	-	500	40	0.179
Biogas IN desulfurizer	0.420	0.080	0.487	0.010	0.003	-	-	333	5	0.174
Biogas IN blower	0.421	0.080	0.488	0.010	0.000	-	-	200	15	0.173
Biogas IN CHP engine	0.421	0.079	0.489	0.010	0.000	-	-	20000	42	0.154
Digestate IN tanks	0.016	0.110	0.871	0.000	0.000	0.000	0.003	101325	40	2.368
Digestate OUT plant	0.016	0.110	0.871	0.000	0.000	0.000	0.003	101325	25	2.368
NaOH IN desulfurizer	-	-	-	-	-	-	-	101325	25	0.001
Na_2S OUT desulfurizer	-	-	-	-	-	-	-	101325	25	0.002
Hot water OUT plant	-	0.112	0.888	-	-	-	-	245097	85	1.958
Air IN CHP engine	-	-	0.233	0.767	-	-	-	101325	25	1.339

Table 4.11 – Mass composition and condition of mass flows

	$\Delta_f H°$ (kJ/kg)	h (kJ/kg)	H (kW)	S° (kJ/kgK)	s (kJ/kgK)	S (kW/K)	e^{ch} (kJ/kg)	e^{ph} (kJ/kg)	e (kJ/kg)	E (kW)
Maize IN plant	-12100	0.00	0.00	5.25	0.00	0.00	10163	0.00	10163	6410
Maize IN reactor	-12100	0.00	0.00	5.25	0.00	0.00	10163	0.00	10163	6282
Water IN plant	-15865	-41.70	-57.92	3.88	-0.14	-0.20	173	0.87	174	242
Water IN reactor	-15865	-40.84	-56.72	3.88	-0.14	-0.20	173	1.77	174	243
Slurry IN plant	-15439	0.00	0.00	4.00	0.00	0.00	1161	0.00	1161	612
Slurry IN reactor	-15439	-1.11	-0.58	4.00	-0.02	-0.01	1161	6.09	1167	615
Biogas IN dehumidifier	-7629	40.21	7.19	7.13	1.72	0.31	16418	-473.88	15944	2850
Biogas IN desulfurizer	-7470	-24.64	-4.29	7.04	1.60	0.28	16868	-502.55	16365	2846
Biogas IN blower	-7494	-24.64	-4.27	7.04	1.75	0.30	16848	-547.65	16300	2825
Biogas IN CHP engine	-7494	22.79	3.50	7.04	0.55	0.08	16848	-142.18	16706	2565
Digestate IN tanks	-15066	60.58	143.42	4.42	0.20	0.47	1246	1.47	1247	2953
Digestate OUT plant	-15066	0.00	0.00	4.42	0.00	0.00	1246	0.00	1246	2950
NaOH IN desulfurizer	-10646	0.00	0.00	1.61	0.00	0.00	2112	0.00	2112	3
Na_2S OUT desulfurizer	-7447	0.00	0.00	4.15	0.00	0.00	8317	0.00	8317	18
Hot water OUT plant	-15865	491.98	491.98	3.88	0.77	1.50	173	22.48	196	383
Air IN CHP engine	0	0.00	0.00	6.74	0.00	0.00	4	0.00	4	5

Table 4.12 – Enthalpy, entropy and exergy flows

The *specific enthalpies* and *entropies per mass unit* have been estimated by using the *software* REFPROP of US NIST (National Institute of Standards and Technology). For the estimation of these quantities, for *maize* dry fraction, it has been necessary to define an *equivalent fuel gas* which would ensure the reckon with such a software, because the latter does not work with the elemental compositions of fuels. In order to ensure the equivalence between the maize dry fraction and the fictitious gaseous fuel it has been verified that the atomic populations and the heating values of the two were identical (exactly equal to 18.7 MJ/kg and to composition in Table 4.13).

Element	y
C	0.436
H	0.074
O	0.489

Molecule	x	y
CH_4	0.458	0.285
CO	0.263	0.286
CO_2	0.215	0.367
H_2O	0.033	0.023
O_2	0.031	0.038

Table 4.13 – Elemental and actual composition of equivalent fuel (dry maize)

The only assumption made is that of considering maize dry fraction as composed only of carbon, oxygen and hydrogen, i.e. neglecting the other elements with a less important weight. The specific *enthalpy* has been therefore calculated as the weighted average, on the mass fractions, of the wet and dry contributions.

$$h_{maize} = \left[h_{water} \left(1 - y_{dry}\right) + h_{eq.F}\, y_{dry} \right]_{maize}$$

The enthalpies, for maize and for all other flows in the plant, have been calculated using REFPROP and as differences between those assessed from the conditions given in Table 4.11 and those evaluated considering the reference conditions (298.15 K and 101325 Pa), in such a way to make the estimates independent from the reference. The exact same procedure has also been used to calculate the *entropies* of the flows. As regards the *physical exergy*, it has been derived from the expression

$$\mathbf{e}^{ph} = \left(h - h_0\right) - T_0 \left(s - s_0\right) \tag{4.3}$$

used for maize and for all other flows. By considering the standard chemical exergy of components of equivalent fuel and of liquid water from Kotas [47] the *chemical exergy* of maize has been assessed with a weighted mean on mass wet and dry fractions. For maize as for all streams the standard enthalpy of formation and the standard entropy were evaluated from the NIST data. *Total exergy* has been assessed as the sum of chemical and physical exergy, and therefore the exergy flow rates have been derived directly from the multiplication of this by the mass flow rate.

$$\dot{\mathbf{E}} = \dot{m}\left(\mathbf{e}^{ph} + \mathbf{e}^{ch}\right) = \dot{m}\,\mathbf{e}_f \tag{4.4}$$

The *m*aize which enters reactors differs from that entering plant just for the maize loss already discussed as shown in Table 4.11 and Table 4.12.

Regarding *feed-water*, it has been considered at the plant inlet a temperature (15 °C) lower than the reference, taking into account that part (in case of use of the liquid fraction of the digestate) or all of this water could come from the water network. For the same reason a pressure of 2.5 bar has been assumed as the average pressure of the aqueduct. Enthalpy and entropy have been calculated through the software and exergy using Equations (4.3) and (4.4). The procedure for the calculation of chemical exergy, for water and the other flows, is the same used for maize and always passes for the values of the standard chemical exergy. The effect of the pump on the water flow at the entrance of the reactor has been evaluated by considering an *increase of pressure* of about 9 bar, taken from the data booklet of some manufacturers of pumps, according to the parameter of flow rate of about 5 m^3/h.

In the case of the *slurry* the problem of calculating of the flow of exergy has been approached as with maize. In this case, however, has not been neglected any fraction of elemental analysis (as the nitrogen and ashes are more abundant in dry fraction and therefore relevant, see Table 4.6) and therefore the *equivalent fuel* with the same atomic population is that reported in Table 4.14.

Element	y
C	0.507
H	0.087
O	0.386
N	0.020

Molecule	x	Y
CH_4	0.456	0.331
CO	0.477	0.604
CO_2	0.000	0.000
H_2O	0.046	0.037
N_2	0.016	0.020
O_2	0.005	0.008

Table 4.14 – Elemental and actual composition of equivalent fuel (dry slurry without ash)

The heating value of equivalent fuel has been assessed to the value of 24.5 MJ/kg. The procedure for the calculation of the thermodynamic quantities is the same already used for maize, except that, this time in the weighted average has been considered the contribution of the ashes. The enthalpy and entropy of the ash has been evaluated with the use of the *coefficients of*

NASA (National Aeronautics and Space Administration) *polynomial expressions* based on JANAF (Joint Army Navy Air Force) data since it has been incalculable with the software used. For the evaluation of the flow of slurry entering the reactor has been considered the *increase in pressure* of 5 bar generated by the pump in accordance with the information from the data booklet of manufacturers of pumps, function of the parameter of flow rate of about 2 m^3/h.

The flow of the *biogas leaving the reactor*s, described in Table 4.8, has been evaluated with the calculation of thermodynamic conditions of temperature and pressure reigning in the reactor via software. The exergy evaluation has been performed as already discussed for the other flows, considering the presence of gaseous species only, obviously.

The composition and flow rate of *dehumidified biogas* has been estimated based on the known information, mass and mole fractions of gas are given in Table 4.15.

Molecule	x	y
CH_4	0.556	0.317
CO_2	0.427	0.667
H_2O	0.002	0.002
H_2S	0.003	0.004
H_2	0.001	0.000
N_2	0.010	0.010

Table 4.15 – Composition of dehumidified biogas

The conditions of temperature and pressure presented in Table 4.11 for the dehumidifier, on the basis of which thermodynamic parameters have been evaluated, have been deduced from the technical catalog of an industrial dehumidifier which considers the operation of the chiller and a *pressure drop* of 40 mm of water column.

The flow of the *biogas leaving the desulfurizer*, described in Table 4.9, has been evaluated with the calculation of thermodynamic conditions of temperature and pressure obtained from a technical report of a similar plant [48].

Regarding the *biogas at the entrance of the CHP engine*, the value of pressure has been estimated from the data from Giommi's technical report [43]. Through the knowledge of the flow rate and of the pressure value has been possible to estimate the rise in temperature consequent to the activity of the blower by reading diagrams of some technical catalogs of blowers.

The estimate of exergy flows of the *digestate* has been carried by considering first of all its composition: this product is, in fact, given by the difference between the feedstock mix introduced in the system and biogas leaving the reactor as shown in Table 4.16.

Element	y_{dry}	y	x
C	0.157	0.016	0.008
H	0.092	0.110	0.661
O	0.722	0.871	0.330
N	0.004	0.000	0.000
S	0.001	0.000	0.000
Cl	0.002	0.000	0.000
Ash	0.025	0.003	0.000

Table 4.16 – Elemental composition of digestate

Neglecting the contribution of nitrogen, sulfur and chlorine an *equivalent fuel* has been estimated to calculate the enthalpy and entropy of the flow; the calculated higher heating value of gaseous fuel and dry fraction without ash taken into account is equal to 9.3 MJ/kg and the compositions are shown in Table 4.17. The contribution of the ash has been taken into account through the use of NASA polynomials and the assessment has been performed as already described for the slurry. The exergetic *flow exiting the digestate tanks* has been evaluated similarly but considering a temperature of 25 °C.

Element	y
C	0.161
H	0.095
O	0.744

Molecule	x	y
CH_4	0.184	0.145
CO	0.090	0.123
CO_2	0.000	0.000
H_2O	0.593	0.523
O_2	0.133	0.209

Table 4.17 – Elemental and actual composition of equivalent fuel (dry digestate without ash)

Thanks to the NIST data for the *sodium hydroxide*, necessary for the capture of sulfur, it has been possible to evaluate the thermodynamic parameters of the flow in input to the desulfurizer. The flow rate has been calculated from known data considering the capture reaction

$$H_2S + 2\,NaOH \rightarrow Na_2S + 2\,H_2O$$

For the byproduct output of the desulfurizer, the water and the *sodium sulphide* has been considered with the composition shown in Table 4.18.

Molecule	y	x
Na_2S	0.684	0.333
H_2O	0.316	0.667

Table 4.18 – Composition of desulfurizer byproduct output

The thermodynamic parameters have been estimated as a weighted mean of the contribution of water (software) and sodium sulfide (NIST data).

The flow of *hot water generated by the CHP engine* has been evaluated by knowing the self-consumption of the thermal power generated by the plant through the equation

$$\dot{m}_{water,H} = \frac{\dot{Q}_{self-consumption}}{c_{water}\left(T_{IN,exc} - T_{OUT,exc}\right)}$$

by taking into account an inlet temperature of 85 °C and an output one of 43 °C for the heat exchanger of the reactor.

Finally, the exergy flow that accompanies the *air required for combustion* has been evaluated taking into account the combustion reactions

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

and less significantly

$$H_2S + \frac{3}{2}O_2 \rightarrow SO_2 + H_2O$$

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$

and considering a ratio of 3.76 between the nitrogen mole and the oxygen one and a 60% air excess consistent with data derived from the data sheet of the Jenbacher gas engine installed in the system.

4.4. Plant economic model

The plant *economic model* has been built according to the approach and methods of Bejan et al. [4] and Peters et al. [49]. To complete a system analysis, in fact, an estimation of the major costs of the plant is important considering various assumptions and predictions referred to economic and technological environment and using *engineering economics techniques.* The *cost* is the amount of money to acquire or produce a good. The *market price* is usually affected not only by production cost, but also by other factors as demand, supply, competition, regulation and subsidies. Very important, especially in a design analysis, is the *cost of a final product.* The total cost of a good is composed by fixed and variable costs. The term *fixed* identified those *costs* that do not change strongly with the production rate like for depreciation, insurance, maintenance. *Variable costs* are those costs that vary more or less directly with the volume of the output like for materials, fuel, labor, electricity.

In this thesis each component of the plant or the plant itself outputs have been considered to have an economic *cost given by* the sum of *fuel cost* (maize silage and pig slurry), *cost of capital investment* and *cost of operating and maintenance* (O&M) for the particular component/plant under exam yielding the output.

4.4.1. Estimating total capital investment

In contrast to fuel and O&M costs, an investment cost is a one-time cost. The capital necessary to purchase the land, build all the required facilities and purchase and install the needed equipment for a plant is called *fixed capital investment* (FCI). The latter is the total system cost assuming an overnight construction, viz. a zero-time design and construction period. The *total capital investment* (TCI) is the sum of the fixed capital investment and other outlays. These ones may be:

- *startup costs*, are mainly associated with design changes that happen after completion of construction but before the system can operate and include labor, materials, equipment and even loss of income while the system is not operating;
- *working capital*, consists of the amount of money invested in items as raw materials, fuels, finished products in stock, cash kept on hand for operating expenses and/or taxes, required to pay for the operating expenses before payment is received by products selling;
- *costs of licensing, research and development*;
- *allowance for funds used during construction*, represents the amount of money disbursed without obtaining any revenue in the period between the beginning of design and the system startup.

The fixed capital investment consists of direct and indirect costs. *Direct costs* are those costs of all permanent equipment, materials, labor and other resources involved in the construction and installation of the permanent facilities. Components of direct costs are purchased equipment (PEC) cost and installation, costs of piping, instrumentation and controls, electrical equipment and materials, land, architectural work and service facilities as water. *Indirect costs* are costs required for the orderly completion of the project like those of engineering and supervision, for developing the detailed plant design and perform supervision and inspection; construction, including contractor's profit and all the expenses for temporary facilities and operations, tools and equipment, home office personnel located at the construction site, insurance; contingencies, to face unplanned expenses due to weather, work stoppages, transportation difficulties.

For the case study, based on the Ravano Green Power (the company that operates the plant) declarations to the press in 2011 [50] a FCI of 4000000 € has been assumed. Clearly this estimate is valid at the time it were developed. Because values like this one may have changed considerably with time due to changes in economic conditions (as inflation or deflation), some method must be used for updating cost data at a past date to costs that are representative of conditions at later time. That is why cost indexes are used. A *cost index* is an index value for a given time showing the cost at that time relative to a certain base time. By knowing the cost at some time in the past, it is so possible to determine the equivalent cost at present by multiplying the original cost by the ratio of the present index value to the index value applicable when the original cost was obtained, i.e.

$$C_{present} = C_{original}\left(\frac{I_{present}}{I_{original}}\right)$$

This way, the FCI of Casalvolone plant has been taken to the value of the reference year for this study, 2013. Through the Intratec Chemical Plant Construction Index the indexes have been estimated to the values of 156.6 and 165.5 respectively for 2011 and for 2013; so, the *FCI* has been evaluated to 4184576 €.

Estimating the *cost of purchased equipment* is the first step in any detailed cost estimation. It is plain that the accuracy of cost estimates depends on the amount and quality of the available information and the budget and time available for making estimates. The best cost estimates may be done directly by *vendors*. The next best sources of cost estimates are those by *experts*, who know costs for professional experience or through calculations using the extensive cost databases often maintained by engineering companies. Another method is that of using *estimating charts* obtained through the correlation of a large number of cost and design data. In a typical cost-estimating chart, when all logarithms of available cost data are plotted versus the logarithms of equipment size, the data correlation results in a straight line in a given capacity range. The slope of this line, α, represents the important parameter known as *scaling exponent*, so, in equation, it gives

$$C_x = C_y \left(\frac{X_x}{X_y} \right)^{\alpha} \tag{4.5}$$

Hence, the purchase cost of an equipment, C_x, at a given capacity or size expressed by X_x, may be estimated when the purchase cost of the same equipment, C_y, at a different capacity or size, expressed by X_y, is known. The variable representing capacity or size is the primary design variable or combination of variables characterizing the size of the equipment in question. As in the absence of other cost information, an exponent value of 0.6 can be used, this approach is known as the *six-tenths rule*. Usually the value of scaling exponent are given for different equipment as a function of capacity range of the equipment.

In case study, since study aim is not to perform an economic analysis of a new facility or to study with precision the real costs of Casalvolone plant but to have a case, as realistic as possible, to build a thermoeconomic analysis and, above all, demonstrate the use of the methodology for the evaluation of uncertainty associated with this type of analysis, for the estimation of the costs in question *simplified relationships* have been used. These expressions are obtained using typical values for the various cost categories; in particular the Equations (4.6) and (4.7) are derived from Bejan et al. [4]

$$TCI = 1{,}47\, FCI \tag{4.6}$$

$$FCI = 4{,}30\, PEC \tag{4.7}$$

So, as a first estimate, it is possible to originate the total capital investment even after assessing the purchased equipment cost. Knowing the fixed cost investment of existent plant, the *TCI* has been estimated swiftly by Equation (4.6) to the value of 6151327 €.

For the evaluation of the *costs of purchased equipment* constituents the nine components, in which the plant has been simplified since the exergy flows analysis, it has been necessary to proceed this way. As it has not been possible to obtain the real cost of the loading systems from operators of the existing plant, these have been derived from information of *screw auger* and *pumps vendors* before being *corrected* using Equation (4.5). For the screw auger, the variable *X* used has been the mass flow rate while for the pumps the volumetric ones; scaling exponents assumed are 0.99 and 0.33 respectively for screw auger and for pumps [49]. All purchased equipment costs results are shown in Table 4.19.

Component	PEC (€)
Screw auger	2607
Pump water	3761
Pump slurry	5181
Digesters	83721
Digestate tanks	51163
Dehumidifier	94452
Desulfurizer	62968
Blower, filter and control	9445
CHP	659859

Table 4.19 – Purchased equipment costs

Digesters and *digestate tanks* costs have been obtained from an *interview with a technician* of EnviTec Biogas as a range of values between 160000 and 200000 € for the reactors and between 90000 and 130000 € for the tanks, because of the variability linked to the inconvenience or various problems such as those associated to the status of the land where plant stands or to the specific requirements of the customer. Therefore, the central value of the interval has been assumed but, because the interviewed technician has interpreted these values as including the costs of the excavation, the land stabilization, but also the installation of the panels and piping, and all necessary ancillary equipment, in fact, these are not true PEC, so, to reach the actual utilized values in the analysis, Equation (4.7) has been used. The cost of the *CHP engine* has been derived from *price lists* of Jenbacher, manufacturer of Casalvolone engine, considering a machine with the same power and efficiency. The purchased equipment costs of the *other three components* have been obtained *by difference*, (they have been allocated according to the power required by the specific component) because no other data were available, by knowing the total value of the *PEC* by Equation (4.7) of 973157 €.

4.4.2. Fuel and operating and maintenance costs

Fuel costs are usually part of the O&M costs but, for their importance in thermal systems are considered separately. For the case study *cost of maize silage* and *pig slurry* (Table 4.20) have been estimated through the information from databases which take into account their variability during the year.

Feedstock	C_F (€/t)
Maize silage	42.8
Pig slurry	3.3

Table 4.20 – Feedstock cost

By dividing these quantities by the heating value of each feedstock, through their sum, the cost of input mix necessary to the system can be achieved to value of 0.039 €/kWh.

The *operating and maintenance costs* may be divided into fixed and variable costs. The fixed O&M costs are composed by costs for operating labor, maintenance labor and materials, overhead, administration and support, distribution and marketing, research and development. The *fixed O&M* costs in the case study have been evaluated by considering those known of an akin plant plus an insurance cost of 2500 €/y while the *variable O&M* costs have been assumed equal to 0.009 €/kWh ($c_{variable}^{O\&M}$) by comparison with those of other plants using renewable and conventional fuels. The value of the fixed O&M cost is 122.5 €/kW ($C_{fixed}^{O\&M}$), a value of an order of magnitude higher than the average of conventional plants.

4.4.3. Cost economic evaluation

As known, an euro in hand today is worth more than a euro received one year from now because the euro in hand now can be invested for the year. Hence, as the cost evaluation of a plant requires comparisons of money transactions at various periods of time, methods are needed to account for the *value of money over time*. If a present value P is deposited into an account earning i percent interest per time period and the interest is remitted at the end of each of n periods, the account will increase to a future value F as expressed by the relationship

$$F = P\left(1+i\right)^{n} \tag{4.8}$$

Interest is the compensation paid for the use of borrowed money, in engineering economy it is expressed in percentage or as a decimal and the unit of time is the year. To calculate the real rate of return of an investment, first of all, the discount rate has been estimated. Indeed, it has been speculated that the plant was paid for the 60% with *equity capital* and 40% with *debt capital*; by considering *interest on the debt* of 3% and a *rate of return on capital debt* of 10%, the *discount rate* has been estimated at 7.2%. The real rate of return, in a first approximation, is given by the difference between the discount rate and the inflation rate. Taking into account an *inflation* of 1.5% the *real rate of return* in question has been calculated to 5.7%.

An *annuity* is a series of equal amount of money transactions happening at equal time periods (year). The annuity term is the time from the beginning of the first time interval to the end of the last time interval. When A euro are deposited at the end of each period in an account earning i percent per period, the future sum is given by

$$\mathrm{F} = A\frac{\left(1+i\right)^{n}-1}{i} \tag{4.9}$$

The *present value* of an annuity is defined as the amount of money that would have to be invested at the beginning of the present period at an effective rate of return per period to yield a total amount at the end of the annuity term equal to the amount of the annuity. By combining Equations (4.8) and (4.9) it results

$$\frac{P}{A} = \frac{\left(1+i\right)^{n}-1}{i\left(1+i\right)^{n}}$$

The reciprocal of this factor is the *capital recovery factor*

$$CRF = \frac{i\left(1+i\right)^{n}}{\left(1+i\right)^{n}-1}$$

that is used to determine the equal amounts A of a series of n money transactions, the present value of which is P. For the case study, a *CRF* of 0.085 has been calculated considering a *useful life* of 20 years.

Thus, the annual *TCI cost* has been evaluated through

$$\dot{Z}^{TCI} = CRF\,TCI$$

obtaining 523314 €/y; while for the *O&M costs* has been used

$$\dot{Z}^{O\&M} = \left(C^{O\&M}_{fixed} + c^{O\&M}_{\text{variable}} H \right) \dot{W}$$

obtaining 193572 €/y, in which *H* is the *operating time* in hours per year, 8000 for Casalvolone plant. This way, the estimate of the hourly costs of the nine components has been performed via

$$\dot{Z}_j = \frac{PEC_j}{PEC} \frac{\dot{Z}^{TCI} + \dot{Z}^{O\&M}}{H}$$

and obtained results are reported in Table 4.21.

Component	Ż (€/h)
Screw auger	0.24
Pump water	0.48
Pump slurry	0.35
Digesters	7.71
Digestate tanks	4.71
Dehumidifier	8.70
Desulfurizer	5.80
Blower, filter and control	0.87
CHP	60.76

Table 4.21 – Components costs

As costs may change during all plant lifetime, levelization can be used to express the relationship between the value of the expenditure at the beginning of the first year and an equivalent annuity or levelized value. The concept of *levelization* is general and is defined as the use of time value of money arithmetic to convert a series of varying quantities to a financially equivalent constant quantity, the annuity, over a specified time interval. *Levelized cost of electricity*, LCOE, is the price at which electricity must be generated to get break even over the lifetime of the project. LCOE is, generally, used in calculating the costs of generation from different sources, it is assessed including cost of fuels together with cost of capital investment and O&M as euro per unit of energy, in fact, electricity generation in the year in question is the quantity used at the denominator of the equation

$$LCOE = \frac{\sum_{t=1}^{n} \frac{\dot{C}_{F,t} + \dot{Z}_t^{TCI} + \dot{Z}_t^{O\&M}}{\left(1+i\right)^t}}{\sum_{t=1}^{n} \frac{\dot{W}_t}{\left(1+i\right)^t}}$$

With a production of 7961326 kWh/y, for the existing plant, has been estimated an *LCOE* equal to 0.19 €/kWh, a value that is amongst the highest compared with other renewable end conventional plants.

4.4.4. Profitability evaluation

An estimation of the expected profit from the investment is essential before capital is invested. In *profitability evaluation* profits and costs that will occur in the future are considered. The associated risks and uncertainties can be significant. In this study three parameters have been considered among all those available in economics: the net present value (NPV), the payback period (PBP) and the internal rate of return (IRR).

Net present value is the sum of the present discounted values of the cash flows over plant lifetime both incoming and outgoing; it represents the amount of money expected at the end of useful life of plant. When it is used for project selection any project with negative present value is rejected and if two projects are mutually exclusive, the one with the highest present value is accepted.

The simple profitability analysis carried out considers an overnight investment cost (that is for the year 0 considering the year 1 as the first year in which the plant starts earning). The capital investment is the only cash outflow in the year of construction while from the first year in which the plant begins to yield products *cash outflows* are the costs of maintenance and feedstocks (949796 €/y). The *revenues* (1751492 €/y) are represented by the multiplication of the generated energy by the *incentive*. The latter has been estimated according to the tariff of current laws: equal to 0.180 €/kWh for plants that use bio-based products (such as maize) and 0.209 €/kWh for plants using bio-based byproducts (such as pig slurry) plus a premium, respectively, equal to 0.040 €/kWh and 0.010 €/kWh to take into account cogeneration benefit if it is present in a small scale cogeneration units and, especially, if the primary energy savings amounted to over 10% [51]. In the case in which bio-based byproducts are used together with bio-based products, with a percentage of the latter not exceeding 30% by weight, the tariff and premium used are those for byproducts, so for Casalvolone plant an *incentive* of 0.220 €/kWh has been assessed. For the investment has been considered a *straight-line depreciation* for 20 years (209229 €/y); taxes are equal to the gross cash flow multiplied by the assumed 34% *tax rate* (201439 €/y). Thus, from net cash flows, the *discounted cash flows* can be calculated by the well-known expression

$$CF_{dis,t} = \frac{CF_t}{\left(1+i\right)^t}$$

and those cumulative ones can be evaluated too as shown in Table 4.22.

Year	CF_{dis} (€)	ΣCF_{dis} (€)
0	-4184576	-4184576
1	567887	-3616689
2	537263	-3079426
3	508291	-2571135
4	480881	-2090254
5	454949	-1635306
6	430415	-1204891
7	407204	-797686
8	385245	-412441
9	364470	-47971
10	344816	296845
11	326221	623067
12	308629	931696
13	291986	1223683
14	276241	1499923
15	261344	1761267
16	247251	2008518
17	233917	2242435
18	221303	2463738
19	209369	2673107
20	198079	2871186

Table 4.22 – Discounted cash flows

Therefore, the net present value is equal to 2871186 €. From Table 4.22 even the *payback period* can be evaluated as about 10 years since it is the length of time required for the cash inflows to recover the original cash outlays required for the initial investment.

At last the *internal rate of return* has been calculated. The IRR method seeks to avoid the arbitrary choice of an interest rate, indeed, it calculates an interest rate internal to the system project in question. This way, the rate which makes the net present value of an investment zero, the internal rate of return, is determined iteratively. For the case study has been assessed to

13.1% by using Excel IRR function. It represents the rate of interest earned on the time varying, unrecovered balances of an investment such that the final investment balance is zero at the end of the plant lifetime.

4.5. Introducing uncertainties

The quality of an analysis depends considerably on the *data gathering* managed. In case study the known real data of the Casalvolone plant have been complemented, when necessary, with *secondary data* or *assumptions*. Data concerning maize and transport related activities were collected by means of *survey on farms* and by *interviews with the farmers*; concerning the pig slurry, data regarding transport activities were collected via *interviews with the owner* of the biogas plant by Bacenetti et al. [36]. So also for information concerning operation of plant, such as biomass consumption, biogas production, electricity and heat requirement, was achieved through *plant monitoring* and *average data* corresponding to the operation in one year (2012) was managed.

All other data have been estimated by the *database*, *data sheets*, *charts*, *tables*, *reports* and materials in general made available by the Department of Agriculture of the University of Milan (2013), with the exception of those taken from the aforementioned *interview with the company manufacturer technician* of the plant. This way, it is easy to understand the degree of *uncertainty* that can characterize data available from so many different sources.

4.5.1. Uncertainties introduced in the study of the digester

In order to have a model such as to apply the proposed method of evaluation of uncertainty, for simplicity, it has been chosen to take account of the *variability in the cost of the feedstock* and *of the components* making up the plant. Just because the *cost of maize silage* and *the pig slurry* have been considered, in economic model, as the mean value between those variables in the course of the year, it has been easy to assess the associated variability. The same can be said regarding the *costs of the digesters* and *digestate tanks* that have been provided from the interview to the company manufacturer technician just as ranges of values. To estimate the uncertainty that accompanies *other plant components*, it has instead resorted to the recommendations in Peters et al.'s text [49]. Indeed, for definitive estimates, based on almost complete data, like that of pig slurry cost, a suggested accuracy is within ±10%; for a scope estimate based on sufficient data to permit the estimate to be budgeted the probable uncertainty is within ±20%; for a study estimate based on knowledge of major items of equipment, like that of desulfurizer, a variability within ±30% has been considered. Hence, for the nine components of the plant, using a *relative uncertainty* the variability of costs is shown in Table 4.23.

Component	C_F	$Z^{TCI}+Z^{O\&M}$	Total
Screw auger	17%	20%	17%
Pump water		20%	20%
Pump slurry	10%	20%	11%
Digesters		11%	11%
Digestate tanks		18%	18%
Dehumidifier		30%	30%
Desulfurizer		30%	30%
Blower, filter and control		30%	30%
CHP		20%	20%

Table 4.23 – Relative uncertainties of plant components costs

The total relative uncertainty of each component has been assessed by considering the three components of cost, feedstocks (fuels), the capital investment and operating and maintenance costs.

5. Case study thermoeconomic Input-Output analysis

Bearing in mind the theory outlined in Chapter 2, and considering all the variables evaluated in Chapter 4 *thermoeconomic Input-Output analysis* has been performed on the model of Casalvolone plant. By considering the theory exposed in Chapter 3, moreover, the *methodology of uncertainty evaluation* has been applied in this type of analysis.

5.1. Existing case analysis

First, the thermoeconomic Input-Output matrix of exergy flows has been built starting from the nine components making up the plant. Then, for the existing case, a thermoeconomic Input-Output analysis has been performed for the evaluation of exergetic and exergoeconomic costs.

5.1.1. Thermoeconomic matrix set-up

Figure 5.1 shows the main *interrelationships amongst the components* of the plant.

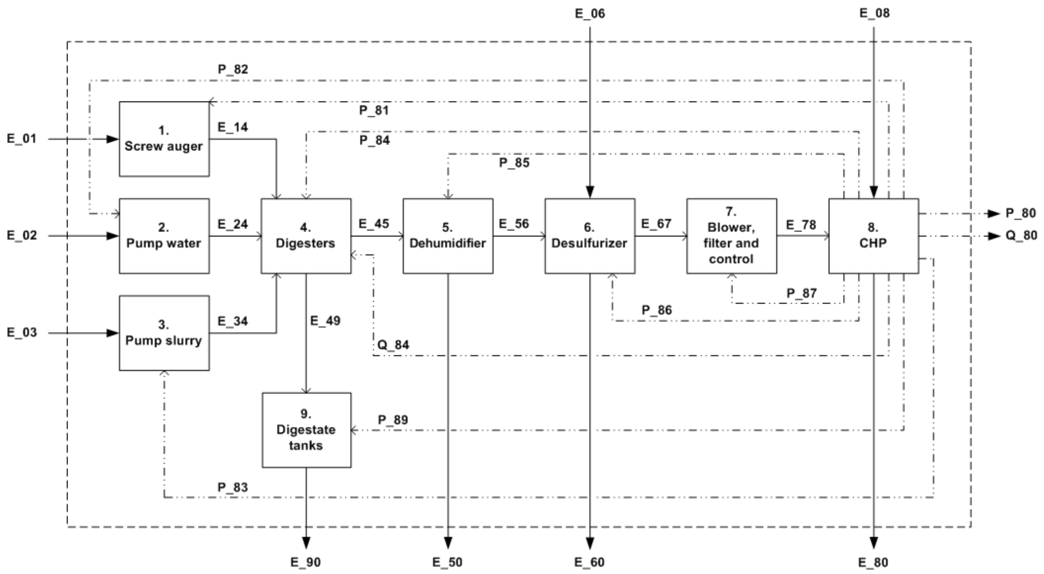


Figure 5.1 – Simplified plant diagram

With the exception of the traced rectangular which represents the boundary of the system, all components are connected by solid lines, those indicating the *material flows*, and dashed lines, those corresponding to the *flows of heat*, Q, and *work*, P, energy. The values of these exergy flows are all known from thermodynamic analysis of the system and are given in Table 5.1. For heat flows of course, the corresponding exergetic one has been evaluated through Carnot factor as already shown in the previous chapters.

Exergy flow	Symbol	Matrix element	Value (kW)
Maize IN plant	E_01	E_{01}	6410
Maize IN reactor	E_14	E_{14}	6282
Water IN plant	E_02	E_{02}	242
Water IN reactor	E_24	E_{24}	243
Slurry IN plant	E_03	E_{03}	611
Slurry IN reactor	E_34	E_{34}	615
Biogas IN dehumidifier	E_45	E_{45}	2850
Biogas IN desulfurizer	E_56	E_{56}	2846
Biogas IN blower	E_67	E_{67}	2825
Biogas IN CHP engine	E_78	E_{78}	2565
Exhaust gas OUT plant	E_80	E_{80}	174
Digestate IN tanks	E_49	E_{49}	2953
Digestate OUT plant	E_90	E_{90}	2950
Water OUT plant	E_50	E_{50}	1
NaOH IN desulfurizer	E_06	E_{06}	3
Na_2S OUT plant	E_60	E_{60}	18
Air IN CHP engine	E_08	E_{08}	5
Power IN screw auger	P_81	E_{81}	65
Power IN pump water	P_82	E_{82}	15
Power IN pump slurry	P_83	E_{83}	20
Power IN reactor	P_84	E_{84}	58
Thermal power IN reactor	Q_84	E_{84}	39
Power IN digestate tanks	P_89	E_{89}	22
Power IN dehumidifier	P_85	E_{85}	15
Power IN desulfurizer	P_86	E_{86}	10
Power IN blower	P_87	E_{87}	2
Power OUT plant	P_80	E_{80}	789
Thermal power OUT plant	Q_80	E_{80}	84

Table 5.1 – Exergy flows for matrix set-up

As it can be seen, each flow is accompanied by two numbers, the first represents the number of the component from which is coming out and the second is the number of the component to which is going in; 0 stands for the environment. In Table 5.1 is even showed the correspondence with the *element of the matrix* in question, evidently when more than a flow is indicated in the same position in the matrix this means that more than a flow rests on that component so it is simply necessary to sum up all the same elements; e.g. the reactor receives electrical and thermal power from the CHP engine, P_84 and Q_84, the element E_{84} is given by the sum of these two contributions. The *matrix* ***E*** is so constructed

$$\boldsymbol{E} = \begin{vmatrix} 0 & 0 & 0 & E_{14} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{24} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{34} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{45} & 0 & 0 & 0 & E_{49} \\ 0 & 0 & 0 & 0 & 0 & E_{56} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_{67} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_{78} & 0 \\ E_{81} & E_{82} & E_{83} & \Sigma E_{84} & E_{85} & E_{86} & E_{87} & 0 & E_{89} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}$$

It is a square matrix 9 × 9, since 9 are the components. By considering also the exergy exchanges with the environment, the *vector of the outputs to the environment* is constructed considering only the exergy flows accompanying products that represent the *actual products* engendered by the production system (final demand), namely electrical and thermal power, the sulphur output from the desulfurization process and the digestate; the vector is therefore made up as

$$\boldsymbol{y}_{env}^{T} = \begin{vmatrix} 0 & 0 & 0 & 0 & 0 & E_{60} & 0 & \Sigma E_{80} & E_{90} \end{vmatrix}$$

The *vector* that represents the *inputs coming from the environment* to the plant (exergetic exogenous resources), instead, is

$$\boldsymbol{v}_{env} = \begin{vmatrix} E_{01} & E_{02} & E_{03} & 0 & 0 & E_{06} & 0 & E_{08} & 0 \end{vmatrix}$$

Moreover, two other vectors can be constructed considering the sums of the elements by row and column (from 0 to 9), those of *total outputs* and *inputs*

$$\boldsymbol{x}^{T} = \begin{vmatrix} \Sigma E_{1j} & \Sigma E_{2j} & \Sigma E_{3j} & \Sigma E_{4j} & \Sigma E_{5j} & \Sigma E_{6j} & \Sigma E_{7j} & \Sigma E_{8j} & \Sigma E_{9j} \end{vmatrix}$$

$$\boldsymbol{w} = \begin{vmatrix} \Sigma E_{i1} & \Sigma E_{i2} & \Sigma E_{i3} & \Sigma E_{i4} & \Sigma E_{i5} & \Sigma E_{i6} & \Sigma E_{i7} & \Sigma E_{i8} & \Sigma E_{i9} \end{vmatrix}$$

By the Equation (2.15) the *technical coefficients matrix* has been estimated

$$\boldsymbol{A} = \begin{vmatrix} 0 & 0 & 0 & 1.083 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.042 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.106 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.001 & 0 & 0 & 0 & 1.001 \\ 0 & 0 & 0 & 0 & 0 & 1.001 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.101 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.293 & 0 \\ 0.010 & 0.062 & 0.033 & 0.017 & 0.005 & 0.004 & 0.001 & 0 & 0.007 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}$$

and so, the *Leontief inverse matrix* has been calculated too

$$(\boldsymbol{I}-\boldsymbol{A})^{-1} = \begin{vmatrix} 1.032 & 0.190 & 0.100 & 1.187 & 1.205 & 1.217 & 1.343 & 3.079 & 1.212 \\ 0.001 & 1.007 & 0.004 & 0.046 & 0.047 & 0.047 & 0.052 & 0.119 & 0.047 \\ 0.003 & 0.019 & 1.010 & 0.116 & 0.118 & 0.119 & 0.131 & 0.301 & 0.119 \\ 0.029 & 0.176 & 0.093 & 1.097 & 1.113 & 1.125 & 1.240 & 2.844 & 1.119 \\ 0.029 & 0.175 & 0.092 & 0.097 & 1.112 & 1.123 & 1.239 & 2.841 & 0.118 \\ 0.029 & 0.175 & 0.092 & 0.097 & 0.112 & 1.122 & 1.237 & 2.837 & 0.118 \\ 0.027 & 0.159 & 0.084 & 0.088 & 0.101 & 0.111 & 1.123 & 2.576 & 0.107 \\ 0.012 & 0.069 & 0.037 & 0.038 & 0.044 & 0.048 & 0.054 & 1.123 & 0.047 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 1.000 \end{vmatrix}$$

The condition number of such a matrix is 37, a relatively low value which involves the loss of one significant digit in results at most. So, the problem is not particularly ill-conditioned.

5.1.2. Exergy cost analysis and evaluation

Through equations from Subparagraphs 2.2.1 and 2.2.2 an *exergy cost analysis* has been performed on the basis of matrixes arrangement explained. The exogenous resources vector consists of exergy flow. For each component the amount of *exergy destruction* has been evaluated and the results obtained are shown in Table 5.2.

Component	E_{des} (kW)
Screw auger	193
Pump water	14
Pump slurry	17
Digesters	1434
Digestate tanks	25
Dehumidifier	18
Desulfurizer	17
Blower, filter and control	262
CHP	1451

Table 5.2 – Exergy destruction

As shown, the major irreversibilities occur in the components where the main energy conversions take place, in the digesters with the conversion from the feedstock mix to biogas and in CHP engine with the conversion from biogas to electrical and thermal power. The other two, in order of importance, major values of exergy destruction are those of the components in which the principal decreases in mass flow rate occurs (due to material loss) with a consequent reduction of the exergy flows.

The *exergetic efficiencies* of the nine components are displayed in Figure 5.2 (see Appendix for all numerical results).

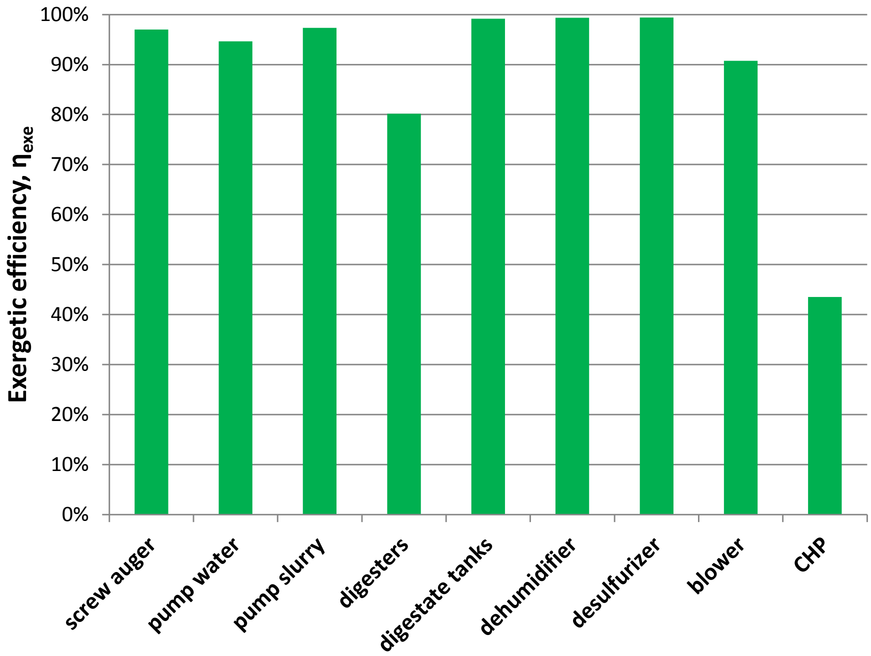


Figure 5.2 – Exergetic efficiencies of plant components

All components have high efficiencies except the CHP engine, in which conversion processes should be enhanced to reduce irreversibilities. Next, by multiplying Leontief inverse matrix by the the exergetic specific exogenous resources vector, the *specific exergetic costs of product per unit of exergy* have been evaluated as presented in Figure 5.3. Each cost, expressed in J/J (or kWh/kWh), is the exergetic expense to produce 1 J (or 1 kWh) of exergy accompanying the output flow of the component in question. The values are all slightly above 1 and, as to be expected, they grow along the chain of the conversions in the system, even if, for the CHP engine the value of the cost is more than doubled compared to others, indicating that the exergetic resources necessary to the engine for the production of electricity and heat (the primary outputs of the plant) are far greater in comparison with the produced energy flows.

Also *costs of fuels per exergy unit* have been estimated for each components as can be seen in Figure 5.4 in which the values are all close to 1.

This way, through Equation (2.7), the *relative cost difference* for all the plant components has been calculated, results are indicated in Figure 5.5.

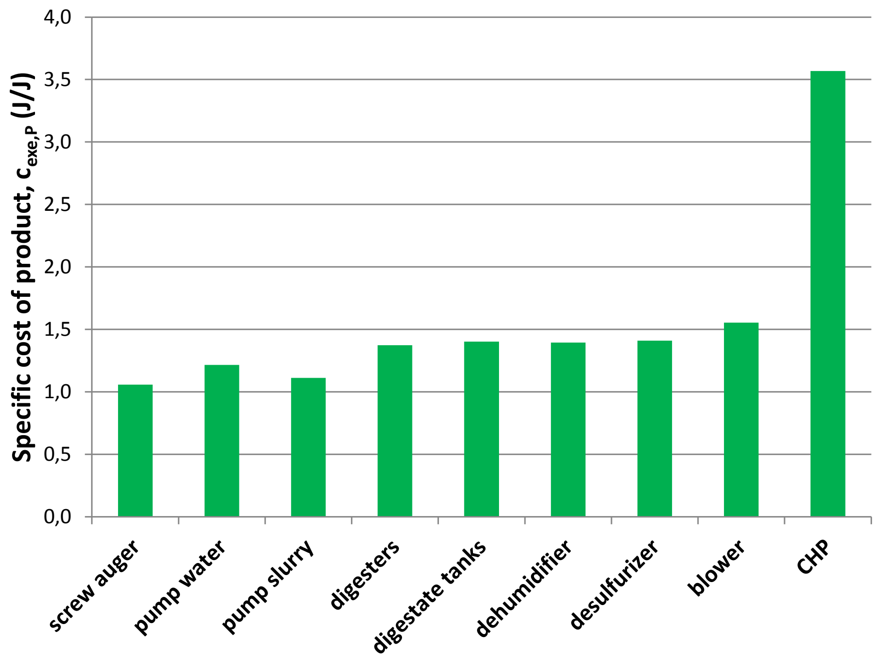


Figure 5.3 – Specific costs of product of plant components

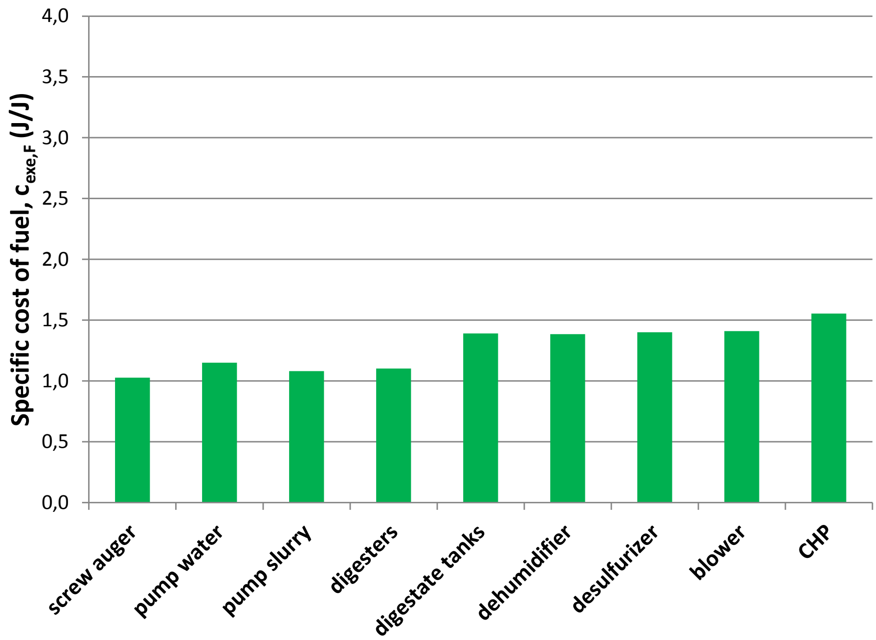


Figure 5.4 – Specific costs of fuel of plant components

The more the value of r is close to zero, the more the difference between the specific costs of product and fuel decreases; this happens for all the components, as expected from the previous Figure 5.3 and Figure 5.4, except for the most critical component, the CHP engine. For the latter the cost of its products is much larger than that of the resources it needs in order to yield its outputs.

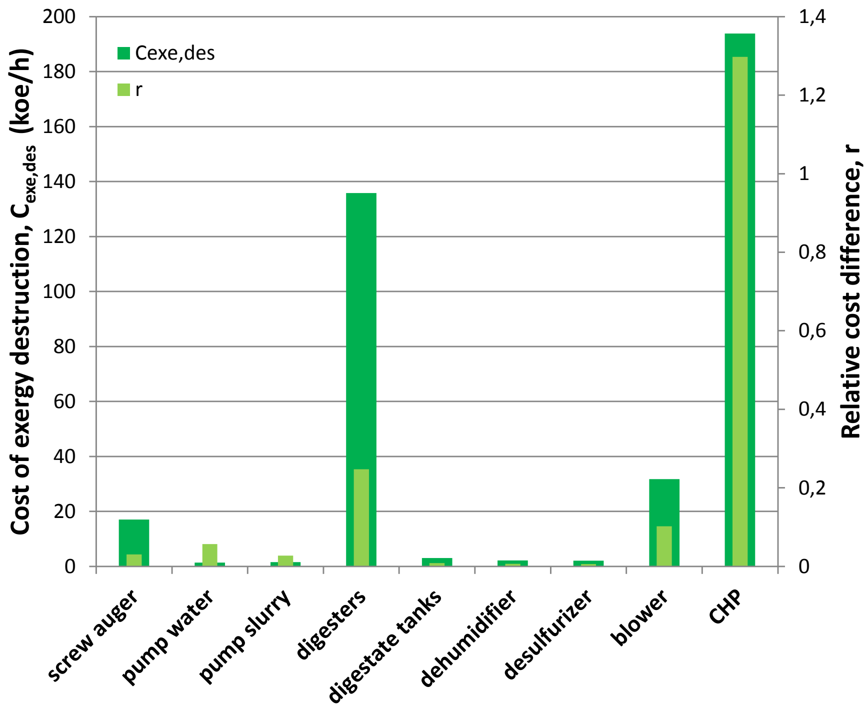


Figure 5.5 – Cost of exergy destruction and relative cost difference of plant components

At last, the *costs of exergy destruction* have been assessed, all values are shown in Table 5.3 and Figure 5.5. For each component, $C_{exe,des}$ is the exergetic cost rate in kW (or koe/h, kilogram of oil equivalent per hours) of the additional fuel which must be supplied to cover the rate of exergy destruction due to irreversibilities.

Component	$C_{exe,des}$ (kW)
Screw auger	198
Pump water	16
Pump slurry	18
Digesters	1579
Digestate tanks	35
Dehumidifier	25
Desulfurizer	24
Blower, filter and control	369
CHP	2254

Table 5.3 – Cost of exergy destruction

The components with evident irreversibilities are those recording the highest costs, so, once again the reactor and above all the engine are the most critical components.

The same analysis has been conducted for the entire plant seen as a whole taking into account the actual output of the system. The *exergy destruction* has been evaluated as sum of all the inefficiencies to the value of 3432 kW. The *total exergy efficiency* of the plant has been calculated equal to 53% and the *cost of the digestate, sulfur and, primarily, of electrical and thermal power generated by the plant* has been estimated to 7271 kW.

The exergy analysis shows undoubtedly that the *CHP engine* is the most critical component, followed by the digesters, as all the indicators, the exergy efficiency, the rate of exergy destruction, the relative cost difference and the cost of exergy destruction suggest to invest in improving the performance of this component and, thus, of the entire plant.

5.1.3. Exergoeconomic cost analysis and evaluation

Through equations from Subparagraphs 2.3.1 and 2.3.2 an economic cost analysis has been carried out too. The *exogenous resources vector* is composed by the cost rates of fuels (feedstocks), of capital investment and O&M expressed as euro per hours, in particular

$$\boldsymbol{v} = \begin{vmatrix} 97.38 & 0.48 & 6.69 & 7.71 & 8.70 & 5.80 & 0.87 & 60.76 & 4.71 \end{vmatrix}$$

In Table 5.4 are shown the values of the *economic costs of products and fuels* of all the plant components.

Component	c_P (€/kWh)	C_P (€/h)	c_F (€/kWh)	C_F (€/h)
Screw auger	0.02	106	0.02	106
Pump water	0.01	2	0.01	2
Pump slurry	0.02	9	0.01	9
Digesters	0.02	138	0.02	130
Digestate tanks	0.03	78	0.02	73
Dehumidifier	0.03	79	0.02	70
Desulfurizer	0.03	86	0.03	80
Blower, filter and control	0.03	86	0.03	85
CHP	0.13	147	0.03	86

Table 5.4 – Cost of products and fuels

The costs analysis of product highlights that the most critical components, the digester and the CHP engine, have the higher costs: the engine presents the largest cost per exergy unit, so, even if its exergy flow output is not higher than that of digesters (biogas and digestate), CHP engine has the largest cost of product per hour; the high value of cost corresponding to the reactors is, instead, due to the considerable exergy flow digesters produce. Similarly, the cost of product of the screw auger (maize silage to the reactors) is high too. With regard to the costs of fuel, the values in Table 5.4 feel the effect of the sizeable exergy flows of maize and of biogas and digestate and then, along the production line of the plant, the effect of biogas exergy flows. Next, the *thermoeconomic variables* have been assessed in accordance with the theory, the results for each component are shown in Table 5.5

Component	C_{des} (€/h)	C_{des} + Z (€/h)	r	f
Screw auger	3.15	3.39	0.03	0.07
Pump water	0.11	0.58	0.31	0.82
Pump slurry	0.24	0.58	0.07	0.59
Digesters	25.86	33.57	0.32	0.23
Digestate tanks	0.63	5.34	0.07	0.88
Dehumidifier	0.45	9.15	0.13	0.95
Desulfurizer	0.47	6.27	0.08	0.92
Blower, filter and control	7.90	8.77	0.11	0.10
CHP	48.67	109.43	2.92	0.56

Table 5.5 – Thermoeconomic variables

where the *costs of investment and O&M* (*Z*) are those in Table 4.21. As it is possible to notice, the costs of exergy destruction reveal that inefficiencies in the critical components lead to higher costs for the system and such effect is more serious for those components that present a greater cost of investment and O&M as shown by the sum of cost of exergy destruction plus Z (thus to the disadvantage of the engine that, in addition to a low efficiency, has a high cost). By observing the values of the *exergoeconomic factor*, three groups of components can be notice:

1. those for which *the factor tends to 1*, like for the dehumidifier; economic savings can be achieved with a reduction of investment costs, since the efficiencies of these components are already high;
2. those for which *the factor tends to 0*, like the screw auger; economic savings can be achieved with an increase of investment costs in order to improve efficiencies (even if the screw auger and the blower are disadvantaged for the presence of material loss);
3. those for which *the factor is in an intermediate position*, the pump of slurry, that has a high efficiency but a cost of exergy destruction disadvantageous, as being calculated on cost of fuels (pig slurry); the CHP engine that presents a low efficiency and a high cost of investment.

The analysis of the entire system has yielded an economic cost of products of 193.1 €/h composed for the 54% by fuel cost and for 46% by investment and O&M cost, since the cost of capital investment and operating and maintenance has been evaluated in the previous chapter to a value of 89.1 €/h.

5.2. Uncertainty evaluation

The relative uncertainty for each plant component exposed in Subparagraph 4.5.1 has been used to characterize the probability distribution around the value of costs of each component. Hence, an *exergoeconomic analysis* has been performed once again *for the existing case* to highlight the *range of values around results*. Finally, a brief sensitivity analysis about assumptions for the definition of exergy destruction cost and for the uncertainty distribution has been carried out.

5.2.1. Exergoeconomic analysis with uncertainty evaluation

Monte Carlo simulations have been used to estimate the uncertainties in the exergoeconomic costs and variables in accordance with the theory offered in Chapter 3. The uncertainty has been introduced as *ranges* because in the interval in which data have been found there is not any value (even less a group of values) that occurs with a probability greater than that of the others. So, also the results are represented with uniform distributions. To evaluate the propagation of uncertainties more than 1000 runs of Monte Carlo method have been required. In Figure 5.6 the results for the evaluation of the *specific cost of product* for each component are shown in €/toe (see Appendix for results in €/kWh).

The results show that always cost values settle in the positions already discussed but as soma *intervals*, not as a unique points. All the possible costs fall in the interval in accordance with the uncertainty of the inputs to the model (fuel and investment costs). The ranges are represented with a kind of box plot in which the whiskers reach the maximum and the minimum values of the interval. The *variability around the mean value* is up to 18% with a minimum to 12% for the pump of the pig slurry, anyway, it is between the relative uncertainties of the input costs.

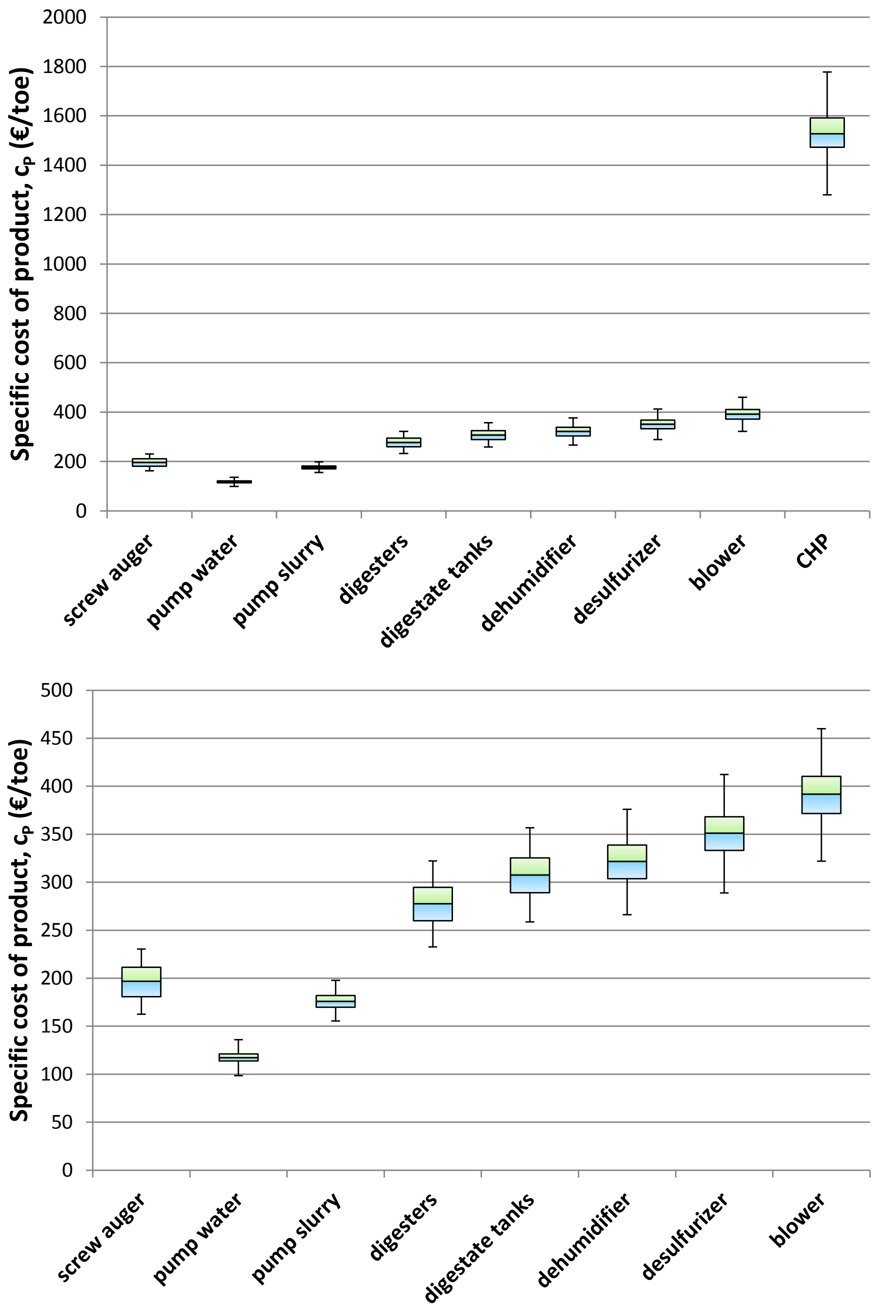


Figure 5.6 – Uncertainty ranges of the specific costs of product

The *hourly costs of products* are reported in Figure 5.7, the relative variability around the mean value is the same of the specific costs and this is true also for the costs of fuel and the cost of exergy destruction but not for the sum of cost of exergy destruction and investment cost, the relative cost difference and the exergoeconomic factor.

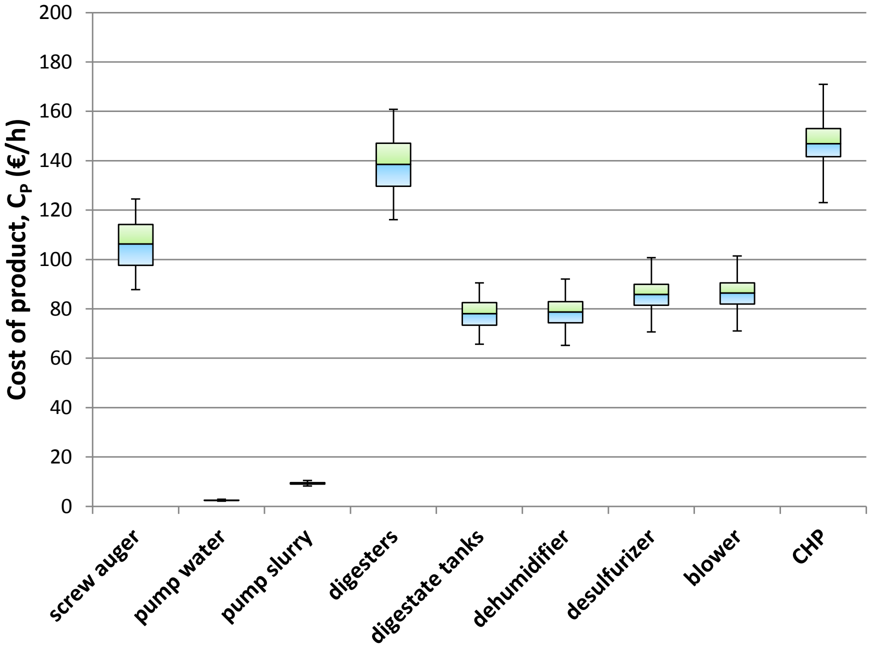


Figure 5.7 – Uncertainty ranges of the costs of product

In Figure 5.8 the *costs per exergy unit of fuels* for each component are displayed.

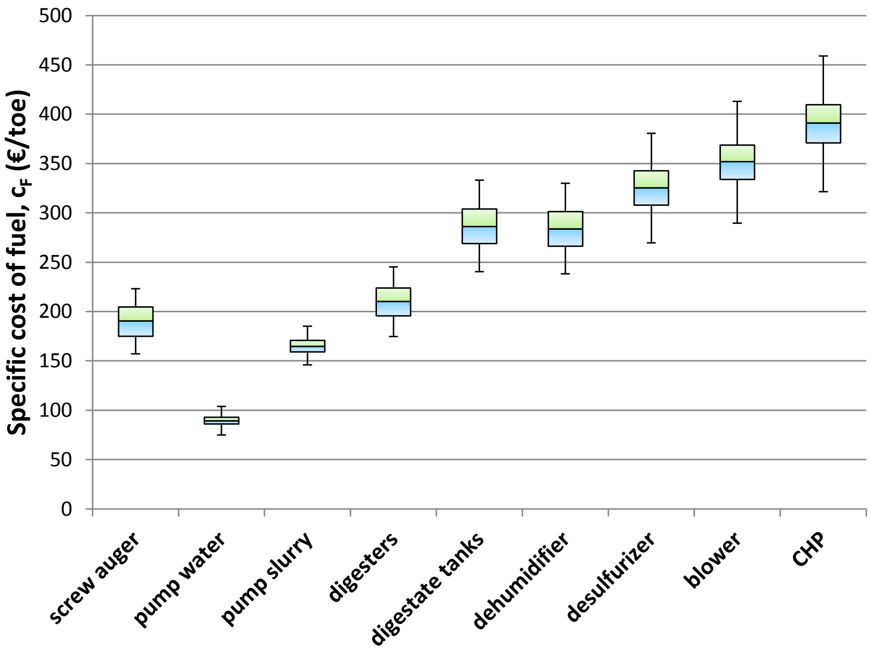


Figure 5.8 – Uncertainty ranges of the specific costs of fuel

Even like intervals, the values show a growing trend along the production line of the system as the quality of the fuels increases from component to component; the fuel of screw auger, the maize silage, has a cost clearly higher than those of water and pig slurry. Then when these costs have been multiplied by the exergy flows that are inputs for the plant the *hourly costs of fuel* have been assessed with their uncertainty intervals as presented in Figure 5.9. That is why the digesters have the highest costs (even if not the largest dispersion own of blower and CHP engine): the exergy flow of the feedstock mix is the highest.

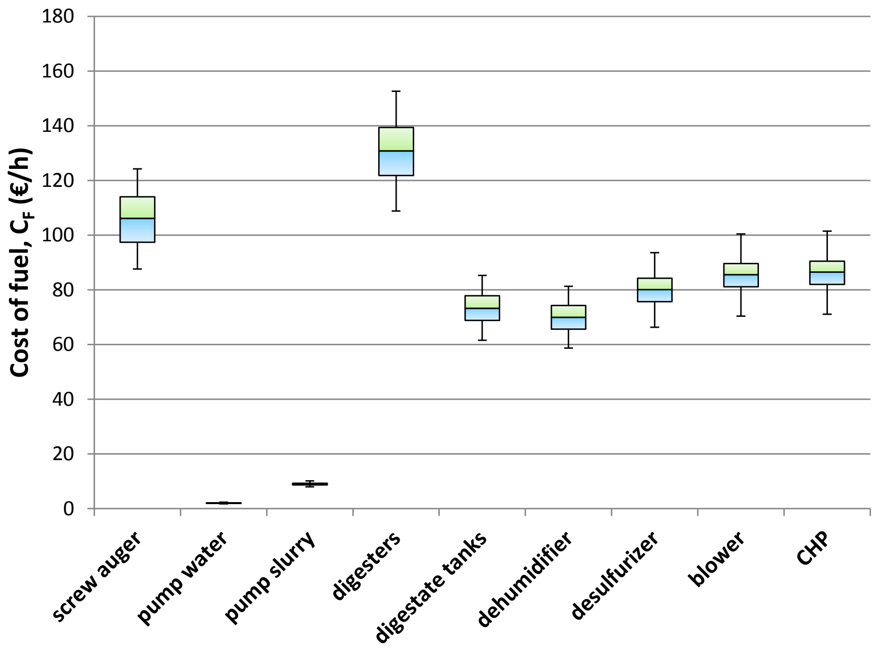


Figure 5.9 – Uncertainty ranges of the costs of fuel

The *costs of exergy destruction* have been estimated with their uncertainty intervals to the value presented in Figure 5.10. The largest values are those of the components in which the exergy destructions are the highest, first of all CHP engine and the digesters (with a relative uncertainty around the mean value of 18% and 17% respectively) and then the blower and the screw auger (18% and 17% of variability). By adding to these costs, those of capital investment and operating and maintenance per hour shown in Table 4.21 accompanied with uncertainties reported in Table 4.23, the values of the *costs of exergy destruction plus Z* have been estimated. Observing Figure 5.11 it is possible to notice the influence of the costs of the components especially for the CHP engine and for the components used in the treatments of the biogas after the digestion.

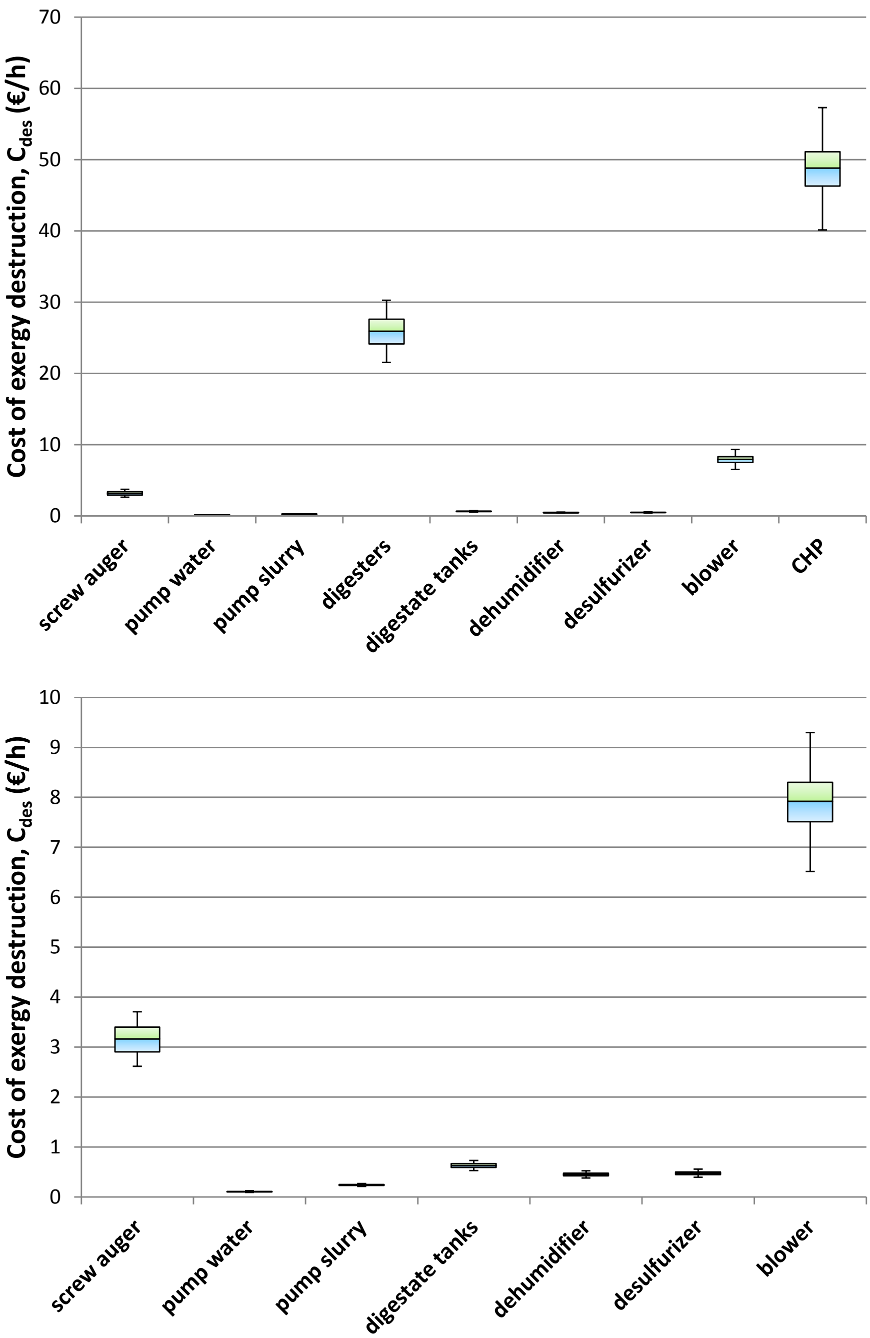


Figure 5.10 – Uncertainty ranges of the costs of exergy destruction

The sum of these costs with different uncertainties also has an effect on the uncertainty of the total variables: intervals are not exactly symmetric, the uncertainties increase for various components, up to 33% of dispersion for the cost values of the dehumidifier since it has been considered the most expensive component among those of biogas treatment; for the digesters, instead, the variability around the mean value decrease to the minimum of 14% amongst all the components.

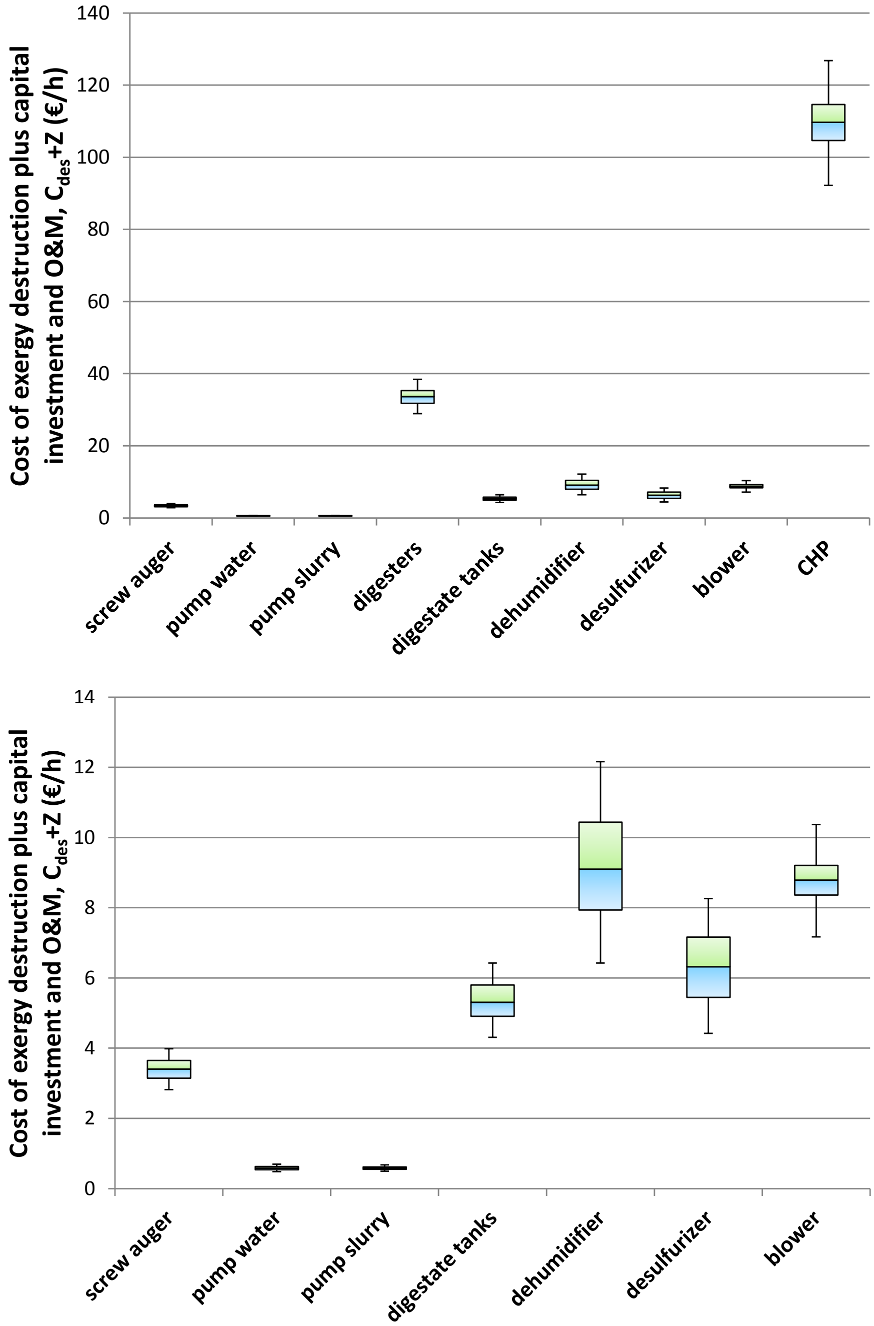


Figure 5.11 – Uncertainty ranges of the costs of exergy destruction and of investment and O&M

The *relative cost difference* and the *exergoeconomic factor* have been estimated too, their values intervals are shown in Figure 5.12 and Figure 5.13.

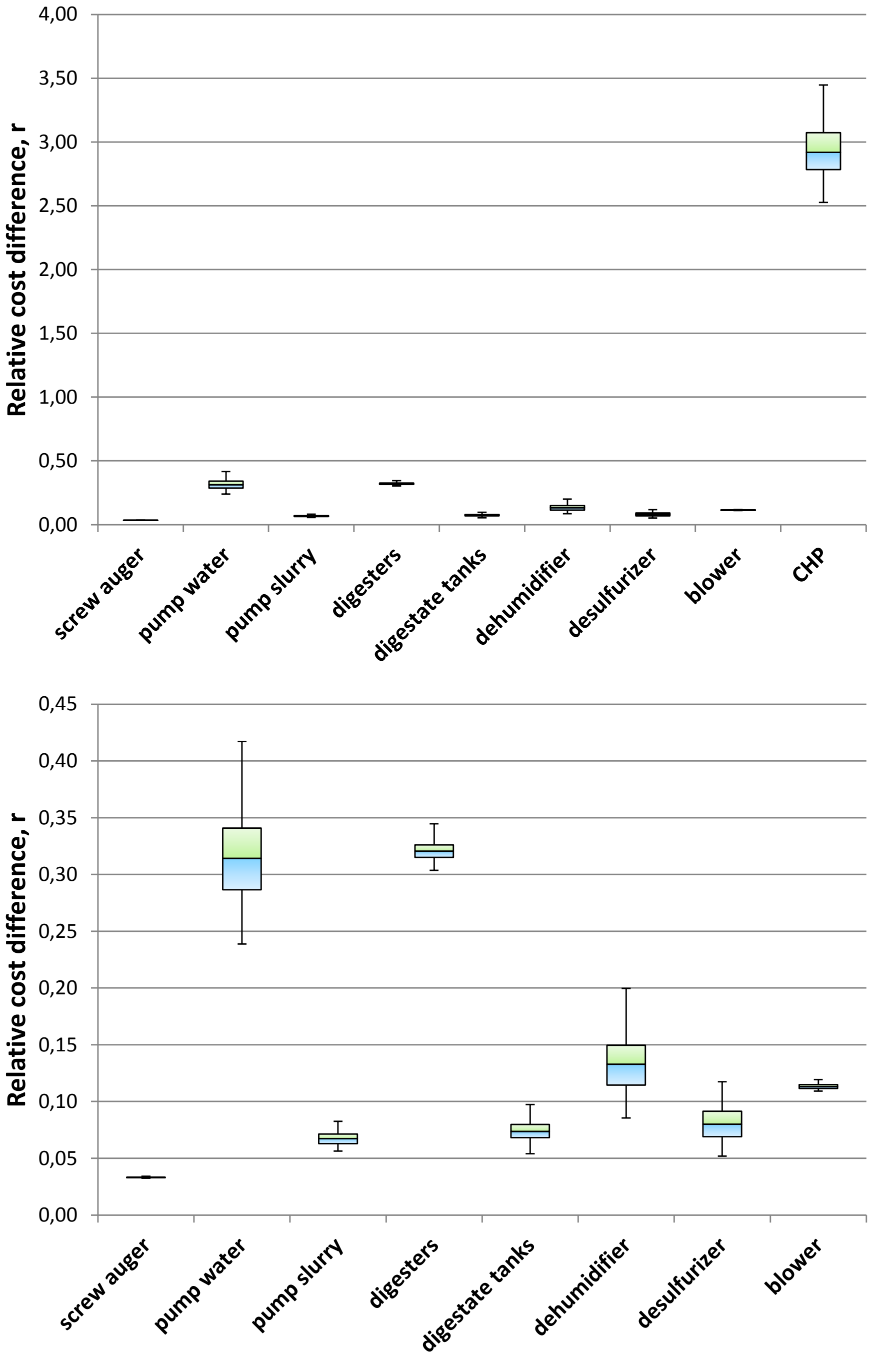


Figure 5.12 – Uncertainty ranges of the relative cost difference

The effect of uncertainties propagations has been ascertained in each component for the relative cost difference:

- the screw auger, the digesters and the blower present a relative uncertainty below 10%, up to 2% for the screw auger;
- the pumps, the digestate tanks and the CHP engine have an uncertainty between 14% and 33%;
- the dehumidifier and the desulfurizer present a high uncertainty over 33% and up to 50% for the dehumidifier, compensated by the fact that the values in question are very low.

Even for relative cost difference and exergoeconomic factor intervals are not symmetric albeit slightly.

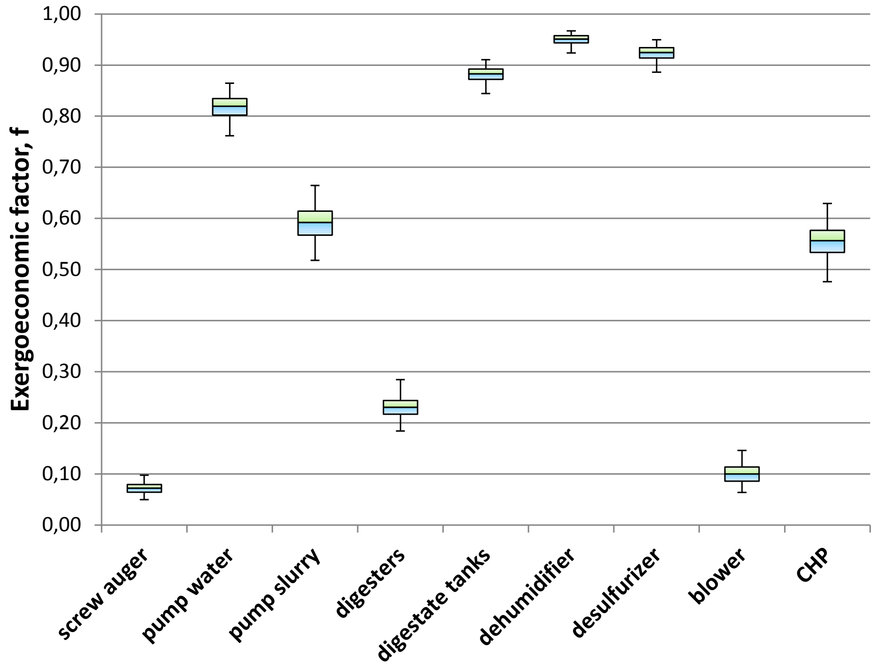


Figure 5.13 – Uncertainty ranges of the exergoeconomic factor

The effect of the propagation of different uncertainties for the exergoeconomic factor has yielded a relatively low dispersion (below 14%) for all components except for the digesters which present a relative uncertainty up to 24% and further for the screw auger and the blower which have relative uncertainties up to 36% and 46% respectively, even here compensated by the fact that the values in question are very low.

The *cost of product of the entire system* has been estimated to the median value of 192.6 €/h with a relative uncertainty of 16%.

Bearing in mind all these considerations, it has been possible to evaluate the needed steps to *enhance cost-effectiveness* of the entire plant. The main component that needs more attention and interest of development is, of course, the *engine* both for its *high cost of investment* and *operating and maintenance* and for that *of exergy destruction* (up to 1014459 € per year) even if it is difficult to imagine that the research to reduce inefficiencies would result in a reduction of engine cost. Next an accurate focus would be directed towards the *digesters* and the *components for the biogas treatment*. Also the information given by the *relative cost difference* underlines these priorities. To reduce the costs of components for biogas treatment, even at the expense of a little loss of efficiency, and to minimize the material losses of maize and biogas from the screw auger and the biogas treatment phase is necessary to improve cost-effectiveness. As well as to reduce the *irreversibilities* in the processes occurring within the digesters and the CHP engine is needed.

5.2.2. Uncertainty due to model assumptions

The *uncertainty linked to the assumptions of the model* has been studied regarding the definition of the *cost of exergy destruction* that, as seen, is a very important thermoeconomic variable. On the basis of theory in Subparagraph 2.1.2 the cost of exergy destruction can be defined as the cost rate of the *additional fuel* that must be supplied to the component in question to cover the rate of exergy destruction or as the monetary loss associated with the *loss of product*. This way, it is a crucial variable of the thermoeconomic models and its definition characterizes the intrinsic uncertainty of the model itself. Such an uncertainty is represented in Figure 5.14 as the possible *range of the values* that the costs of exergy destruction can take for each component.

Neither of the two assumptions used to define the cost is strictly satisfied and these definitions are just approximations of the average costs rate associated with exergy destruction. The use of the specific cost of fuel or of product respectively gives a lower or a higher estimate with the *actual exergy destruction cost* being somewhere between the two within the ranges. As it is observable, the change in the assumption is not significant for various components except for the two in which *material loss* occur and the other two in which *inefficiencies* are relevant. In both cases the process irreversibilities affect the value of the exergy destruction and accordingly the ranges of the cost of exergy destruction so much so that the intervals are as wider as the exergy destruction in the component in question is higher. For the CHP engine, in which the inefficiencies are the largest, the variability around the mean value is high to 39%, for the digesters is equal to 11%, for all the other components is under 5%.

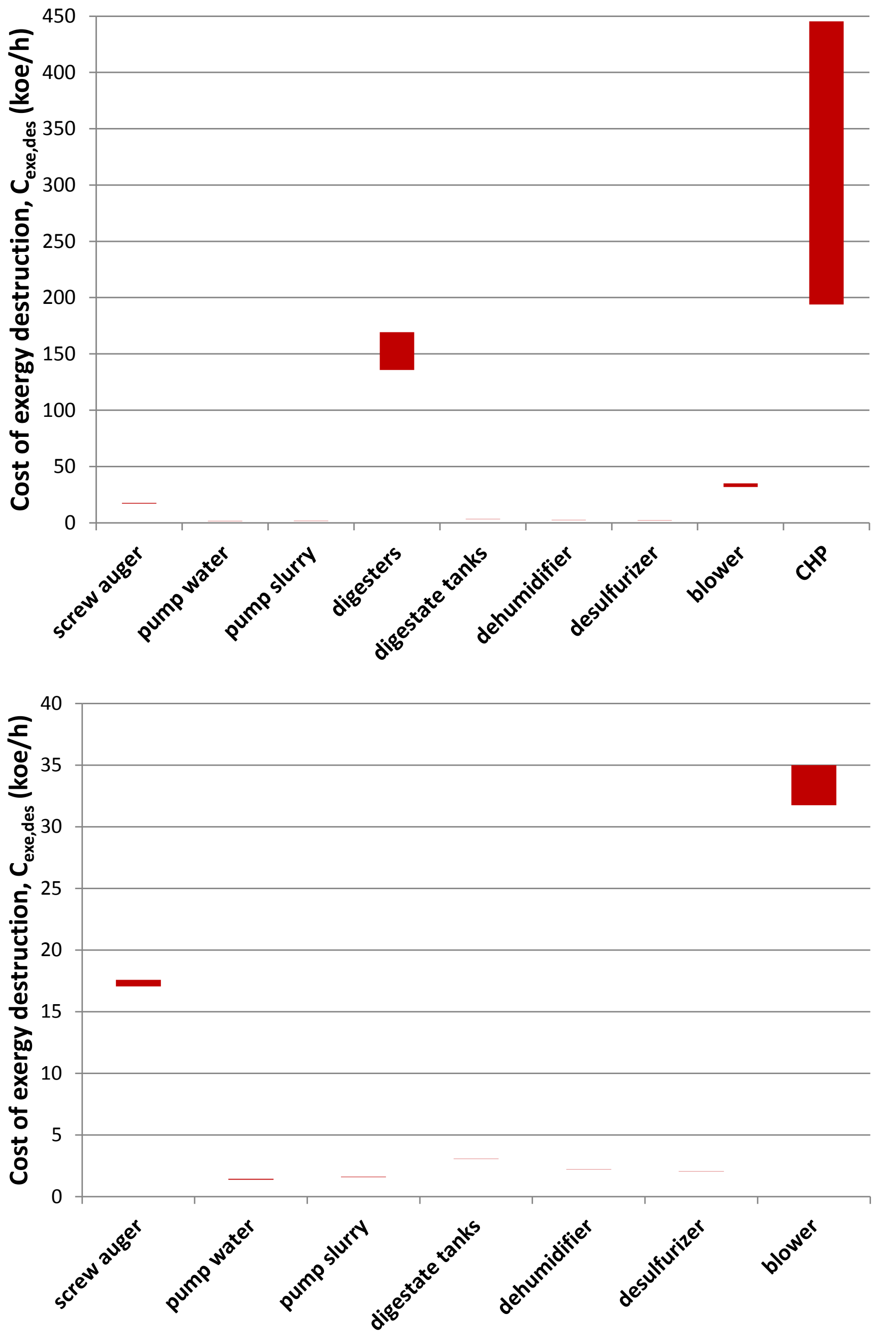


Figure 5.14 – Uncertainty ranges due to the different definitions of exergetic cost of exergy destruction

To consider, in addition to this *intrinsic uncertainty of thermoeconomic model*, the *uncertainties due to the variability in exogenous resources vector*, is very interesting as can be seen in Figure 5.15.

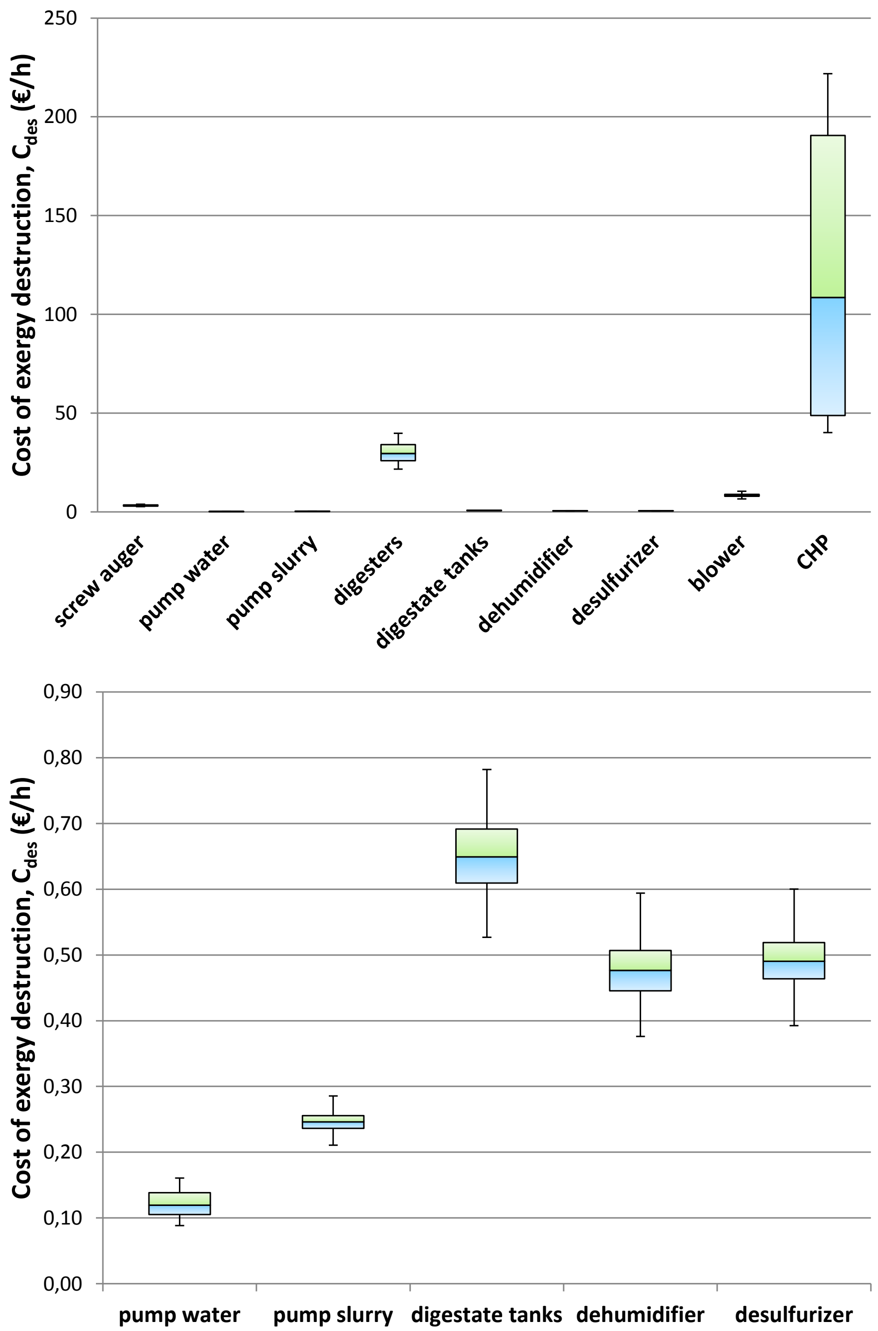


Figure 5.15 – Uncertainty ranges due to the different definitions of economic cost of exergy destruction

In fact, the CHP engine show a very high variability (up to 86%) so that the information provided is insignificant as all values between 40 and 222 €/h could be the actual cost of exergy destruction for that component. Even for the digesters the uncertainty is high but lesser (up to 33%), for the other components is under 32%. Hence, when efficiency is low and consequently the exergy destruction is large, to know the value of exergy destruction cost rate becomes very hard.

Another important aspect analyzed is the *arbitrary assumption about the uncertainty distribution*. Up to now the only distribution analyzed has been the uniform distribution (since no information has led to think that, for example, there is a greater probability that the values of the results fall in the middle of the intervals) but, some academics [7] suggest the use of the *Gaussian distribution* for the uncertainty evaluation. Through Monte Carlo simulations it is possible to simulate this distribution characterizing the dispersion of a parameter with a mean value and a standard deviation. Whit the relative uncertainty available in Table 4.23, the percentage of the total uncertainty has been used to generate the standard deviation and the central value of the cost has been utilized as mean value. Figure 5.16 presents a comparison between the calculation of the cost of products with a uniform and a normal distribution.

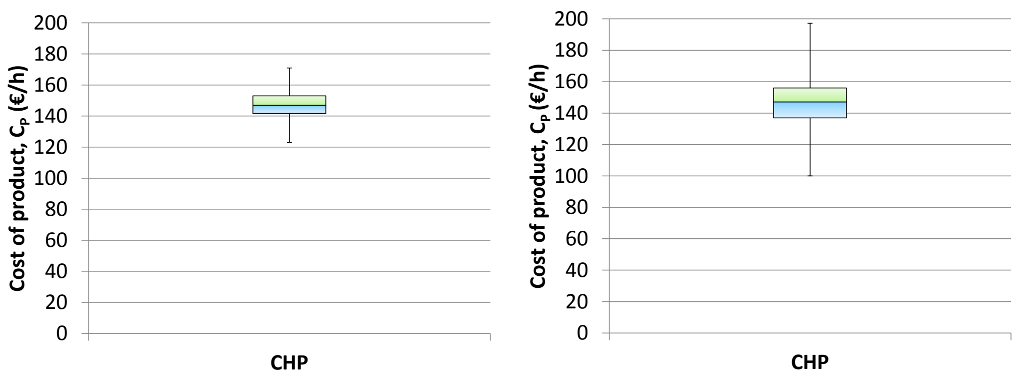


Figure 5.16 – Uncertainty ranges due to the different distributions: uniform (on the left) and Gaussian (on the right)

In a simply way, the Gaussian distribution, by taking into account also the costs that have a very low probability to happen, broadens the uncertainty ranges. These considerations are valid for an analysis ex post the construction of the plant with the little information available; in a context ex ante plant building all the possible costs are known by the designer and so, when there are uncertainties, the real distributions are known too.

5.3. Design optimization

At the conclusion of the work, a *design optimization of the system* in question has been performed. The aim of such a study is the research of the *optimum mix between the two feedstocks* of the plant, the maize silage and the pig slurry, that guarantees the *economic optimum*, with the lowest costs and the largest profits and the *thermodynamic optimum*, through a thermoeconomic Input-Output analysis, with the lowest resources consumption. Thus, the chosen *parameter for the optimization* is the *mass fraction of maize*, the only input of the plant considered together with the slurry. The search of the optimum would permit the plant to work in the most efficient way and with the lowest cost, for instance, with the lowest use of maize as this fuel is more expensive than the slurry. The optimization has been carried out with the limit of the *constant plant principal output*: in each configuration the electrical power produced is constant to 995 kW as the thermal power to 1076 kW. The *12 configurations considered* cover all the possible feedstock mix from 0% of maize (equal to 100% of slurry) to 100% of maize (0% of slurry). In the first configuration there are not costs of maize, screw auger and pump of water and exergy flows regarding these components are equal to zero. In the last configuration there are not costs of slurry and pump of slurry, so, exergy flows at the turn of this component are equal to zero.

5.3.1. Economic considerations

The economic analysis shown in the previous paragraphs has been reapplied for all the configurations, the *cost analysis* has yielded the results presented in Figure 5.17 varying percentage of maize introduced in the plant. For the *first five configurations* the capital investment is larger than that of the last seven configurations because of the higher costs for the digesters and the digestate tanks. In fact, in the first five configurations, as the maize silage utilized is modest, a lot of slurry has to be used to obtain the constant power output. This results in a *greater volume of the feedstock introduced* in the reactors or rather in an *increase of the number of reactors* for the plant. In the configuration with 100% slurry, 829 t/d of pig slurry are required, so the feedstock volume must be divided into 6 digesters and the produced digestate in the same number of tanks. For the configuration with 5% of maize silage, the number of reactors has been estimated equal to 4, 3 for those with 15%, 25% and 35% of maize, while from 45% to 100% of maize 2 reactors are sufficient. The costs analysis show that there is not a predominant configuration which permits large reduction of costs, excluding the first five configuration with a total cost from 223 to 198 €/h, the *configurations from 45% up to 100% of maize input are equivalent* with a total cost of 193 €/h.

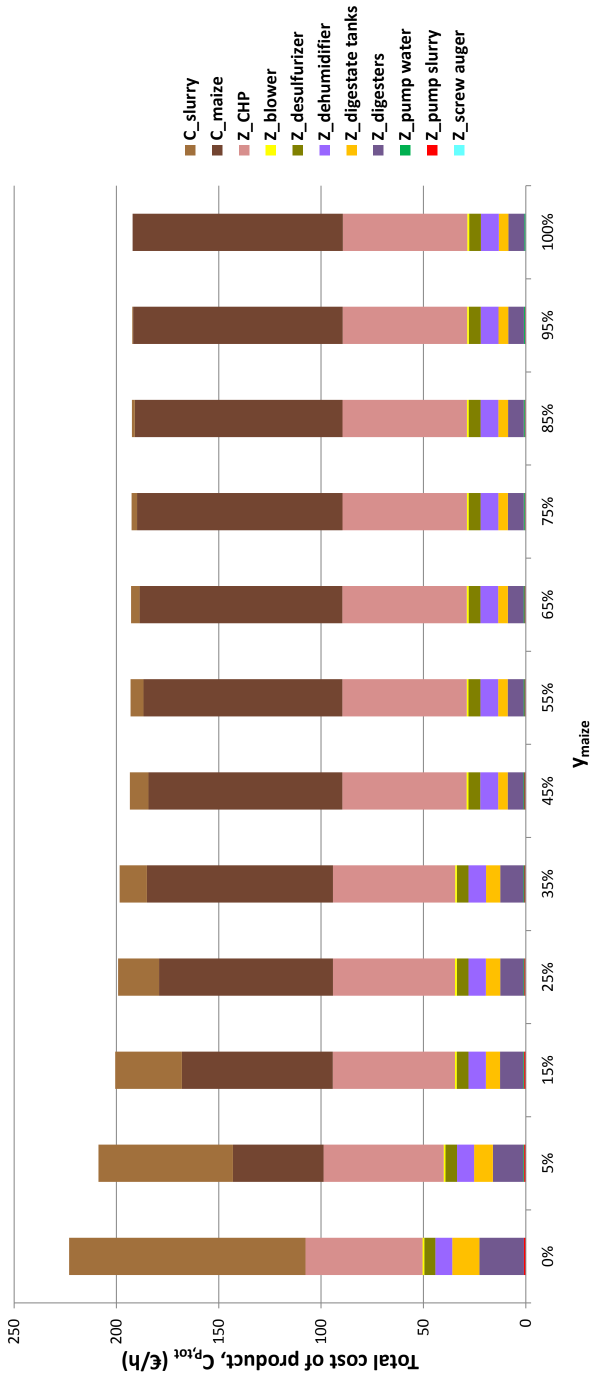


Figure 5.17 – Cost composition

In order to find the economic optimum, also a *profitability analysis* has been performed for each configuration and results are reported in Table 5.6.

y_{maize}	NPV (€)	PBP (y)	IRR (%)	LCOE (€/kWh)
0%	1262831	15	8	0.212
5%	1724098	13	10	0.203
15%	1956274	12	11	0.199
25%	1956622	12	11	0.199
35%	2636251	10	12	0.199
45%	2868625	10	13	0.194
55%	2871186	10	13	0.194
65%	2869236	10	13	0.194
75%	2869561	10	13	0.194
85%	2869942	10	13	0.194
95%	2870510	10	13	0.194
100%	2871727	10	13	0.194

Table 5.6 – Profitability indicators and LCOE

Even this analysis confirm that *from 45% of maize input all configurations allow to reach the highest profits*. For the first five configurations the *incentives* considered have been estimated to the lower value of 0.209 €/kWh since the premium for the cogeneration cannot be given for the failed primary energy saving of 10% for these plants. The configuration with 55% of maize (the existing case) and that with 100% of maize input are those for which the net present value is higher albeit slightly. The *levelized cost* of electricity has been also evaluated as displayed in Table 5.6 and the results conform to what already seen.

5.3.2. Thermoeconomic considerations

With a *thermoeconomic analysis* of all the plant as a whole for each configuration has been assessed the trend of the *exergy destruction* as shown in Figure 5.18. No central information can be inferred from such a flat trend except that of the main value, round 295 koe/h (about 3430 kW) equal to about 4 times the net electrical power of the plant. Figure 5.19 presents the trend of the *exergetic efficiency* and shows that the configuration with the highest efficiency is that with 0% of maize and then the trend decreases. The trends of *exergetic cost of product* and *economic cost of product* with the associated uncertainties intervals have been calculated and exposed in Figure 5.20. Both present the lowest costs with increasing the amount of maize introduced in the plant. The exergetic cost tends to the value of 600 koe/h (about 7000 kW). The ranges of the economic costs have been evaluated as explained in the previous paragraphs to obtain a relative uncertainty not bigger than 17% (for the configurations with 95% and 100% of maize input).

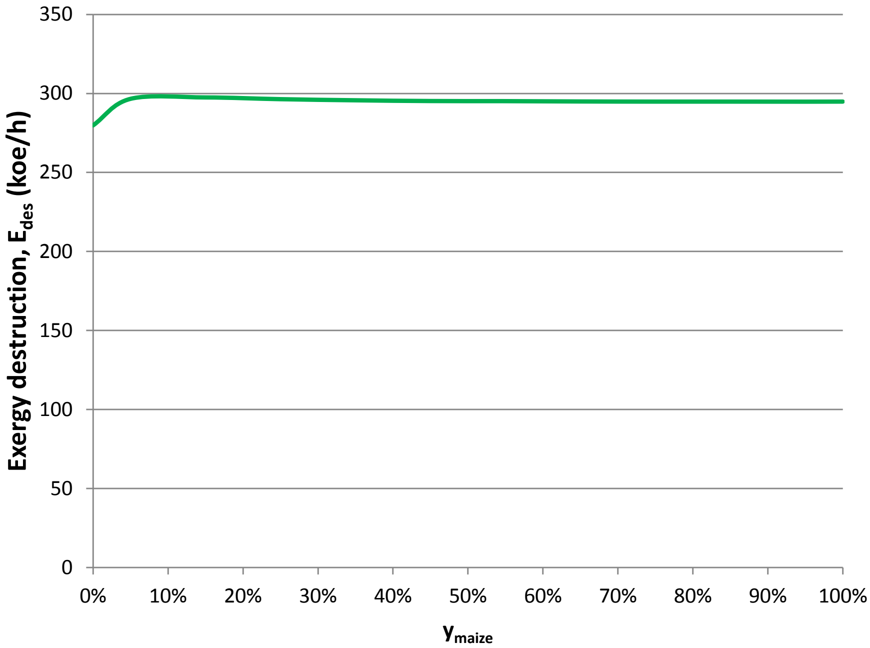


Figure 5.18 – Exergy destructions

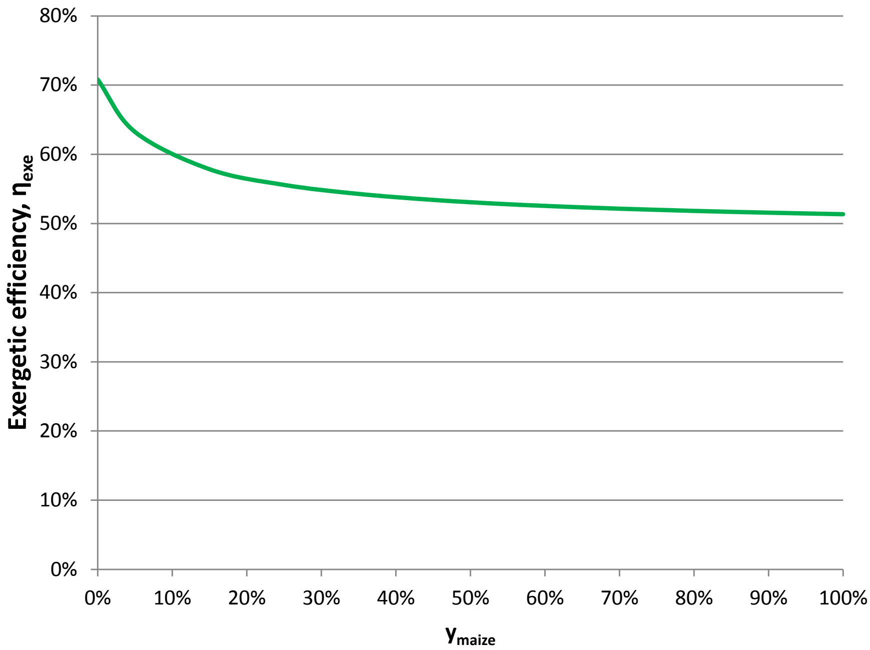
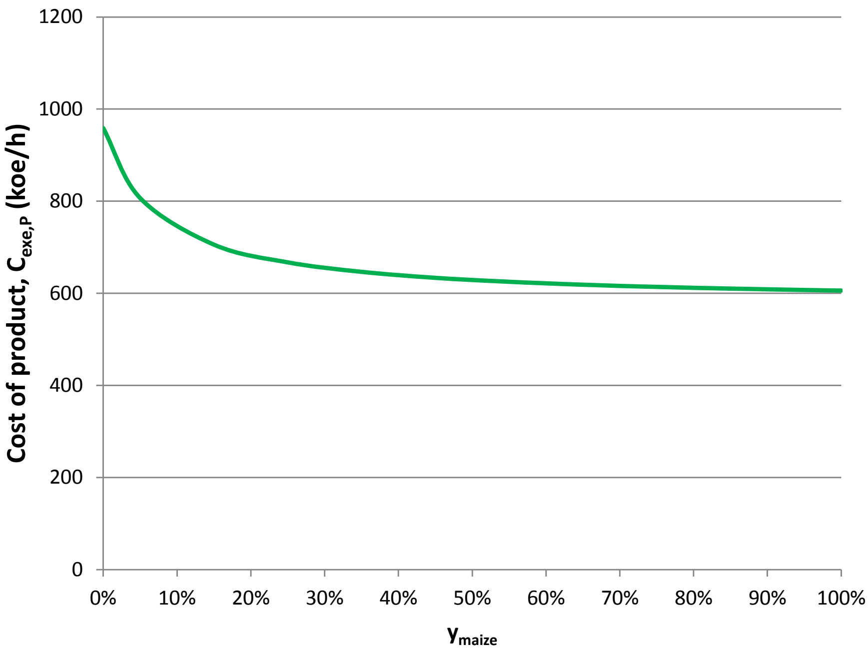


Figure 5.19 – Exergetic efficiencies



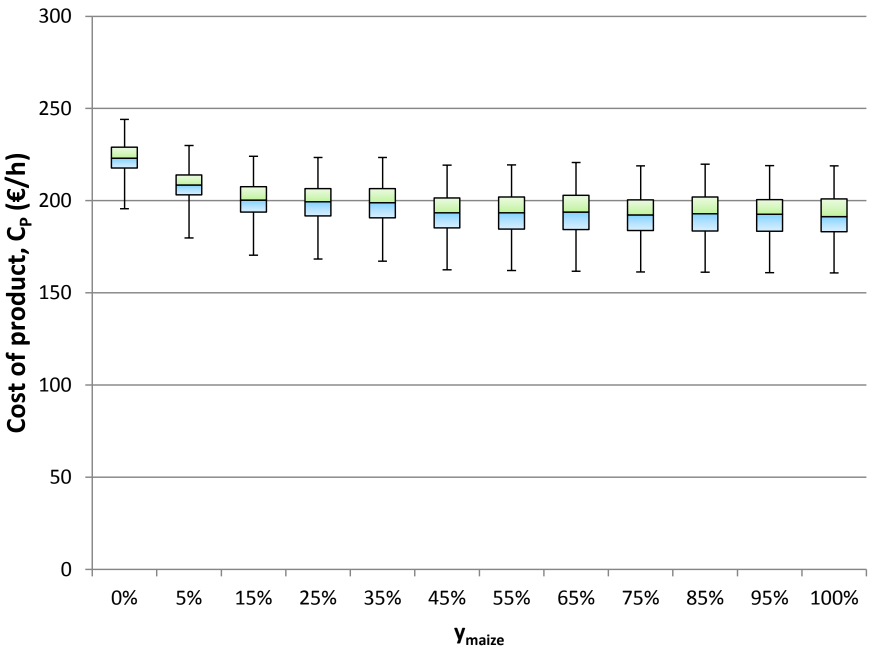
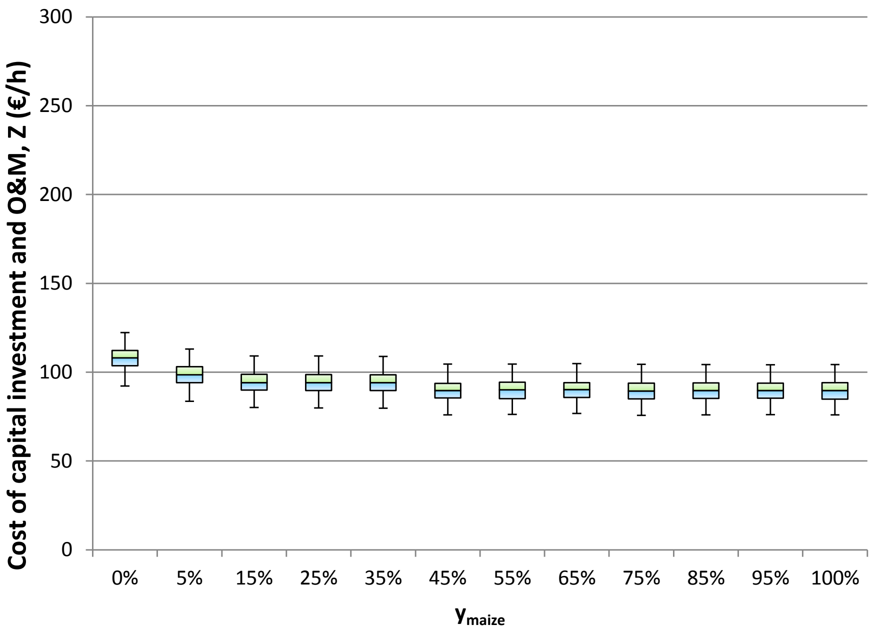


Figure 5.20 – Exergetic and economic costs of product

At last, the values of the two components of the economic cost of product have been estimated and presented in Figure 5.21: the *cost of fuel* and *of investment and maintenance*. The cost of product is given by the sum of these two.



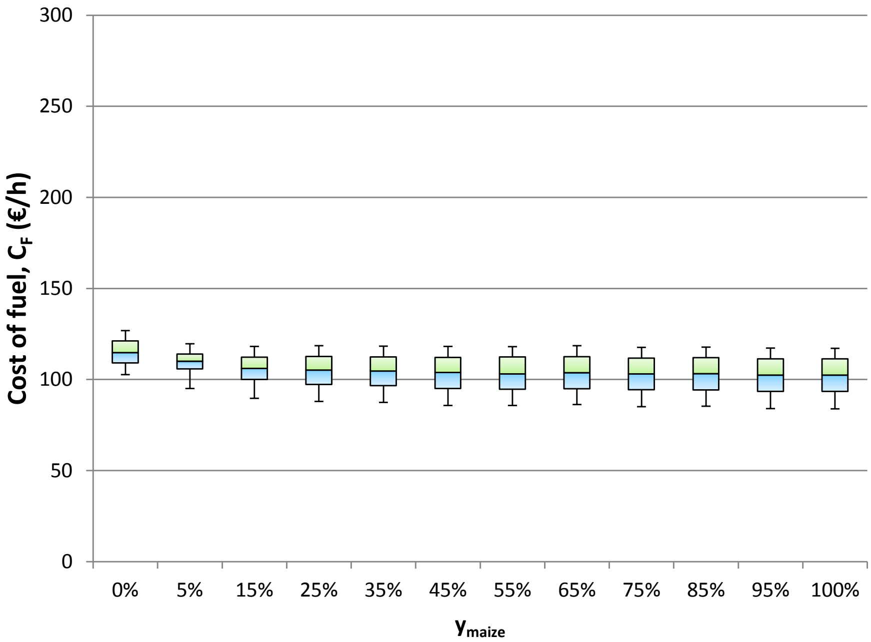


Figure 5.21 – Costs of capital investment and O&M and of fuel

So, it is possible to conclude that all the configuration from 45% of maize input upward are equivalent for the minimization of the costs both exergetic and economic. Even economic analysis confirm this conclusion, nevertheless, with a comparison with Figure 5.19 an *intermediate configuration* (the existing case 55% of maize input) is preferable not to reduce too much the efficiency of the system. Moreover, the choice of a configuration with 55% of maize input instead of 100%, for instance, allows the use of a greater amount of slurry. The *energy valorization* of such an *agricultural byproduct* is important also to *avoid* an *uncontrolled release* into the atmosphere *of methane*.

6. Conclusions

This thesis presents a *method for the uncertainty evaluation and the uncertainty propagation assessment in thermoeconomic Input-Output analysis*. The context in question is that of the valorisation and the description of the natural, exergy resources necessary in production chains to yield products. All the available instruments, the exergetic, economic and statistical analyses have been utilized to elaborate the methodology.

The concept of available and destroyed energy, together with the economic concept of cost have been used in the thermoeconomic analysis to estimate the cost of the product of a system starting from the system dataset and accessible information. Since each type of data presents some uncertainty, the main statistical instruments to describe it have been provided. The problem to study uncertainty propagation has been solved through the application of various *Monte Carlo simulations* in order to evaluate the uncertainty in the results of the Input-Output analysis, the costs and the thermoeconomic variables. Monte Carlo technique is an approach very fast and reliable whenever to handle a huge amount of data is possible.

Also thanks to the application of the method in a case study, it has been possible to verify how thermoeconomic analysis is of central importance for the characterization of the resources needed to produce goods. However, it must be accompanied by a consistent uncertainty analysis to assess the variability linked to results and to perform a *critical evaluation* of the achieved information. In fact, the assumptions about the model affect the validity of the results, so that they need to be assessed case by case carefully remembering that there is more *dispersion* where the exergetic inefficiency is higher. Systems in which the exergy destruction is larger, and in which the exergetic efficiency is lower, are those on which it is necessary to invest to reduce *irreversibilities*.

The uncertainty evaluation can be useful also in the problems of thermoeconomic *optimization* since the characterization of intervals instead of fixed point may lead to different conclusions in the cost minimization process.

It is important to underline that, even if in this work the application of the methodology based on Monte Carlo simulations has been applied at that part of the matrixes arrangement of Input-Output analysis identified as economic resources vector, the *formalisation* of the method for the analysis is *general*. In principle, uncertainty affects every kind of data, thus variability and dispersion can characterize the exogenous resources and the final demand vectors up to spread in the Leontief inverse matrix. This way, the described methodology for Input-Output analysis may be applied in different fields as well as that of Life Cycle Assessment, for the supply chains analysis, thanks to its versatility. In effect, once established the uncertainties in input data, by Monte Carlo simulations, the uncertainties that have reached the output results may be estimate, so that an accurate *data gathering phase* and some *good computing capabilities* are the key points for a successful implementation of the method.

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Appendixes

Exergy cost analysis, existing case

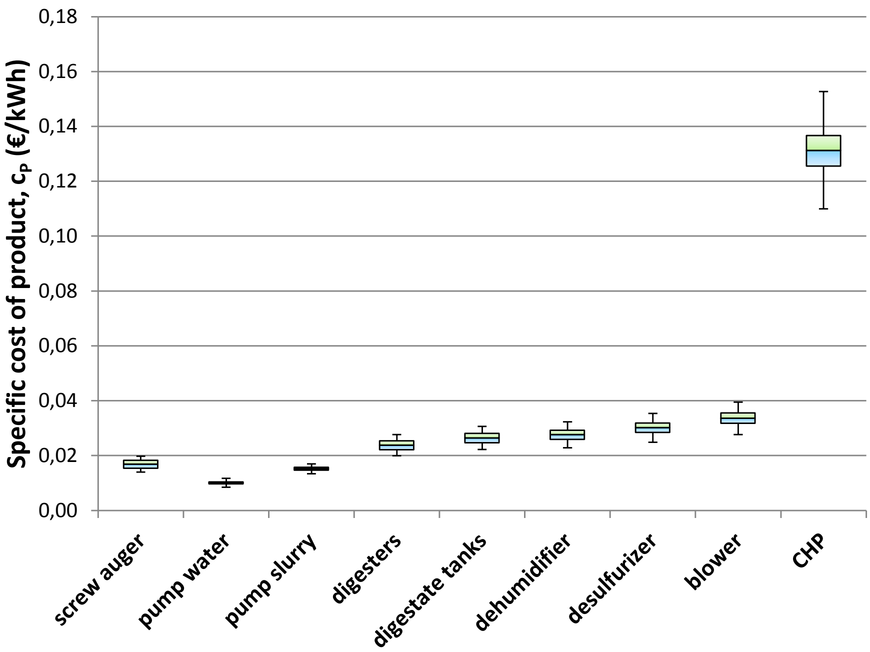
Component	E_{des} (kW)	η_{exe}
Screw auger	193	97%
Pump water	14	95%
Pump slurry	17	97%
Digesters	1434	80%
Digestate tanks	25	99%
Dehumidifier	18	99%
Desulfurizer	17	99%
Blower, filter and control	262	91%
CHP	1451	44%

Exergy destruction and efficiencies of plant components

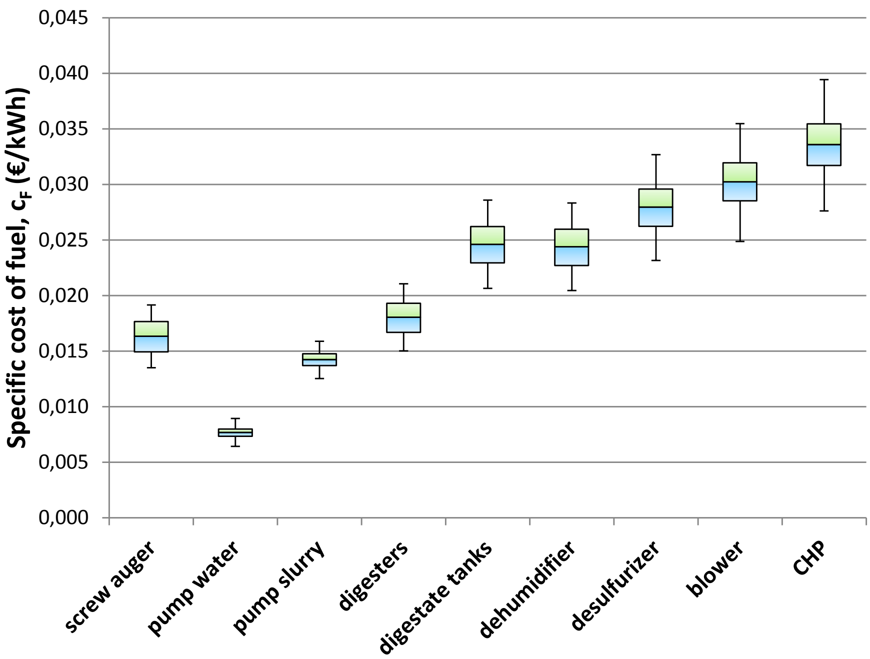
Component	$c_{exe,P}$	$C_{exe,P}$ (kW)	$c_{exe,F}$	$C_{exe,des}$ (kW)	r
Screw auger	1.06	6642	1.03	198	0.03
Pump water	1.22	295	1.15	16	0.06
Pump slurry	1.11	683	1.08	18	0.03
Digesters	1.37	7968	1.10	1579	0.25
Digestate tanks	1.40	4134	1.39	35	0.01
Dehumidifier	1.39	3966	1.38	25	0.01
Desulfurizer	1.41	4005	1.40	24	0.01
Blower, filter and control	1.55	3986	1.41	369	0.10
CHP	3.57	3991	1.55	2254	1.30

Costs of products, fuels, exergy destruction and relative cost difference

Uncertainty evaluation, existing case



Uncertainty ranges of the specific costs of product



Uncertainty ranges of the specific costs of fuel