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COMPARATIVE STUDY OF ENVIRONMENTAL EVALUATION ASSESSMENT USING EXERGETIC LCA IMPLEMENTED IN EXISTING SOFTWARE AND A NOVEL EXERGETIC APPROACH DURING THE EARLY DESIGN PHASE

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ABSTRACT

Current environmental evaluation analysis methods such as LCA require detailed information about the studied product or process. This leads to uncertain or wrong results when applied during the early design phase. As a result all the design choices must be made before performing such environmental analysis, consequently such methods are not truly design tools. The proposed exergetic approach offers an appropriate solution for an environmental evaluation during the early stages of the design process. A key aspect of this exergetic approach is a combination of a classical exergy and dimensional analysis. In previous works, the exergetic approach has been compared using LCA eco-indicator 99 (H), as the LCA method is a widely used and accepted method. This article aims at further validating the exergetic method by comparing it to the LCA exergetic method implemented in existing, widely spread, software. The comparison of the two approaches is done through a case study which is part of a project that is in the early design stage. This work is a part of the development of a tool that provides a model-based approach of the entire engineering design process.

Keywords: Exergy, environmental evaluation analysis, LCA, validation

1 INTRODUCTION

The knowledge required for a full Life Cycle Assessment (LCA) most often does not match the knowledge present at the early stages of product development. Indeed, during those stages, very few parts are known for a fact which makes a reliable full environmental assessment difficult to obtain.

The development of tools providing repeatable methods based on generic metric aggregating several aspects of the impact assessment is essential for providing correct environmental assessments right from the early stages of product development.

The goal of this article is to further compare the introduced exergetic method to widely implemented methods. It should be mentioned that the introduction of the exergetic approach combined with Π numbers is part of a very ambitious program aimed at developing a model-based approach of the entire engineering design process. Exergy is used as a combined metric derived from the basic metrics of the SI system. Π numbers are part of the Dimensional Analysis Theory [1], [2] and this constitutes a powerful tool to transform the design space into a design space called metric space. This result comes from the branch of mathematics named topology. One fundamental result of topology is that a metric space is the best suited one for comparison [2], [3]. These two elements are part of a model-based project implemented in computer tools and should support more a intensive use of computers in the early phases of engineering design. The present article participates in the construction of an ontology layer dedicated to environmental and life cycle assessments. The global ontology system will be designed using a set of ontology layers mapped together using the Simantics language [4]. Simantics has similarities with Protégé and its ontology language OWL.

Figure 1 describes a potential combination of ontology in simanitcs.

We consider that the above digression is a necessary step to put our research in perspective of our global project involving several researchers.

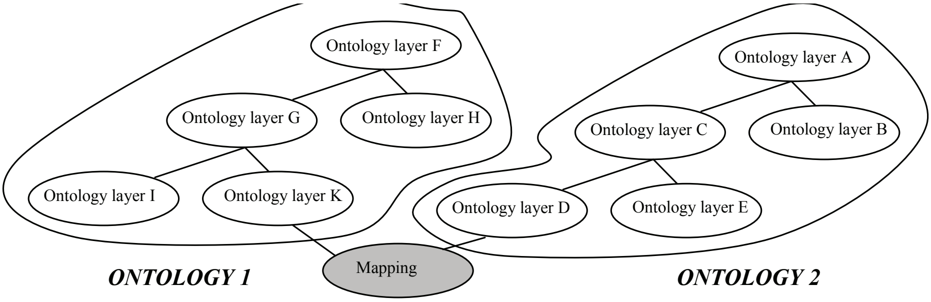


Figure 1: Mapping between ontologies of engineering design

Life Cycle Assessment (LCA) is a widely used environmental impact assessment method, even though its scientific reliability has been criticized. A comparative study between the exergetic method and LCA using Eco-Indicator 99 (H) has been performed in a previous work [5]. Recently LCA has been coupled with exergy in the Cumulative Exergy Demand (CExD) indicator in the software SimaPro 7.1.8. This software is the basis for the comparative study performed in this paper.

The rest of this paper is organized as follows:

Section 2 presents the state of the art of exergy research which started developing in the 1950's with research by Rant [6] and others such as Wall [7].

Section 3 gives an overview of LCA and exergetic LCA implemented in software. The method is based on the research of Bösch *et al.* [8].

Section 4 is a presentation of the exergetic approach developed by Coatanéa [2] using dimensional analysis as a central tool for the comparison and evaluation of concepts. The method is further presented in the case study.

Section 5 presents the case study of the article. Two systems are compared using both exergetic LCA and the developed exergy approach.

Section 6 and 7 contain the comparison and discussion of the results. Section 6 summarizes the results. Future research works for a complete early design phase environmental assessment tool are presented in Section 7.

2 STATE OF THE ART IN EXERGY RESEARCH

Exergy can be regarded as a measure of useful energy by the definition of Rant [6], it is stated to be the maximum amount of work that can be produced by a system or a flow of matter or energy as it comes to equilibrium with a reference environment. Wall [7] defines exergy as work, or ordered motion, or ability to produce work as opposed to energy which is motion or ability to produce motion. Exergy is expressed in Joules (J) or ML^2T^{-2} using the international system of fundamental quantities with (M) Mass, (L) Length and (T) Time. Whereas energy is always conserved as per the first law of dynamics, exergy is consumed in real world processes as stated in the second law of thermodynamics [9]:

$$\delta Ex = T_0 \sum \Delta S \tag{1}$$

Ex = Exergy loss due to irreversibility inside the system (J)
T_0 = Temperature of the surroundings (K)
S = Entropy (J/K)

2.1 Exergy as an environmental metric

According to Seager and Theis [10], there are six broad categories of sustainable metrics: financial, thermodynamic, environmental, ecological, socio-political and aggregated metrics. Exergy is classified as a thermodynamic metric rather than an environmental metric. Multiple propositions have been made for environmental metrics such as a simple waste exergy accountancy [11] or exergy of mixing [12].

2.2 Exergy calculation

The formulas on which most exergetic calculations are based can be found in Szargut [9]. Exergy has four basic forms, kinetic, potential, chemical and physical. In the case of an environmental study, only the chemical and physical exergies present an interest.

Physical exergy:

$$Ex_{Ph} = m[(h - h_0) - T_0(s - s_0)] \tag{2}$$

m: mass (kg),
T_0: temperature of the environment (K),
h: specific enthalpy of the flow (J/kg),
h_0: specific enthalpy of the flow at temperature T_0 and pressure P_0 (J/kg),
s: specific entropy of the flow (J/(kg.K)),
s_0: specific entropy of the flow at temperature T_0 and pressure P_0 (J/(kg.K))

Standard chemical exergy:

$$Ex^0_{ChP} = G^0 + \sum_i \left(\frac{n_i}{n_p} Ex^0_{Chi}\right) \tag{3}$$

Ex^0_{ChP} : standard chemical exergy of a compound (J/mol),
G_0: Gibbs free energy of formation of the compound from the elements (J/mol),
ni: number of moles,
Ex^0_{Chi} : standard chemical exergy of the ith reactand required to form np moles of the product compound (J/mol),
ni and np: stoichiometric balancing numbers of the appropriate chemical reaction.

An approximation of the environmental impact can be made using the exergy of mixing which represents the portion of the chemical exergy due to material transfers or changes in composition. This can be a measure of the potential chemical change due to the introduction of any pollutant in the environment as argued by Coatanéa *et al.* [13].

Exergy of mixing:

$$Ex_i^m = n_i R T_0 \ln\left(\frac{y_i}{y_i^0}\right) \tag{4}$$

Ex_i^m : exergy of the composition-dependant component (J),
n_i: total number of moles of the species,
y_i: activity in the thermodynamic system under consideration,
y_i^0: reference activity in the appropriate environment (sea, earth crust or atmosphere).

3 EXERGY APPLIED TO LCA – CUMULATIVE EXERGY DEMAND

3.1 – Presentation of LCA

Life Cycle Assessment is the most commonly used approach during the design process to determine the final environmental impact [14]. LCA is usually performed as a four-step process: 1) scoping, 2) inventory analysis, 3) impact assessment and 4) improvement assessment. During the third stage, an array of impact category indicators such as Eco-Indicator 99 (EI 99), Cumulative Energy Demand (CED) and Cumulative Exergy Demand (CExD) can be used [15].

The LCA software SimaPro describes the four stages as 1) characterization, 2) damage assessment, 3) normalization and 4) weighting. Only the first step is required by ISO standards, not all assessments include the last three steps. As described in the introduction to implementing the LCA software, the results must be thought out and communicated in a careful and well-balanced way as not to cause confusion as to their meaning [16].

3.2 – Shortcomings of LCA

As described in 2.2, exergy can be considered as a thermodynamic metric and research has been done to include exergy in environmental metrics. LCA and other systems analysis methods lack a uniform metric basis which leads to difficult comparisons or expressions of different impacts or requirements [11].

As the method is descriptive, the amount of data necessary to complete a single study is enormous. Moreover, it relies on databases which contain some data that is unverifiable and unreliable. It does not offer support during the early stage of design as all the product components have to be known before an extensive environmental impact assessment can be performed. LCA is also often seen as an external part of the design process as separate software and knowledge is required. Millet et al. [17] discuss the lack of integration of LCA with commonly used design tools such as CAD software.

There are multiple indicators that can be used to evaluate the impact after the life cycle inventory. The results greatly vary when one indicator is used over another one [8]. Each indicator focuses on a different amount of resources and characterizes them differently, for example Eco-Indicator 99 considers that water is an inexhaustible resource.

3.3 LCA combined with exergy

The idea of combining LCA and exergy has been suggested before; Cornelissen [18] proposed to extend LCA with an Exergetic Life Cycle Analysis (ELCA). It is shown that in the case of a zero-exergy process LCA can be replaced with ELCA.

The LCA software SimaPro proposes the Cumulative Exergy Demand (CExD) indicator. It depicts the total exergy removed from nature that was necessary to provide a product, therefore it's the exergy of all the resources required. Bösch *et al.* [8] provide the basis for CExD calculation for 2630 ecoinvent product and process systems. The results are shown for eight impact categories: fossil fuel, nuclear, hydropower, biomass, other renewable, water, minerals and metal.

The CExD method is also the basis for the Cumulative Exergy Extraction from the Natural Environment (CEENE) method which produces more consistent results [19]. It has not yet been implemented in LCA software.

3.4 Discussion of possible results obtained with such a method

The CExD method implemented in SimaPro provides the total exergy that needs to be removed from nature in order to provide a product and that is no longer accessible for future exploitation. The authors of the CExD indicator note that several aspects are not taken into account in CExD such as social demand of a resource or its technical availability or scarcity. As the availability of a resource is not evaluated in the indicator, fewer assumptions are made and create a more reliable database. Results obtained with the CExD indicator were compared with three major indicators, Cumulative Energy Demand (CED), Eco-Indicator 99 and CML 2001. The impact categories of CExD differ from other indicators but Bösch *et al.*[8] concluded that it is a useful LCA component.

4 EXERGETIC APPROACH

4.1 Exergy calculation – dimensionless numbers

In order to evaluate the material and resource consumption efficiency and environmental impact, several dimensionless numbers have been introduced by Coatanéa *et al.*[13] and further developed by Medyna *et al.* [5]. The creation of Π numbers transforms the general design space into a metric space and thermodynamic and environmental metrics as described below.

The concept of exergy requires different types of inputs and outputs:

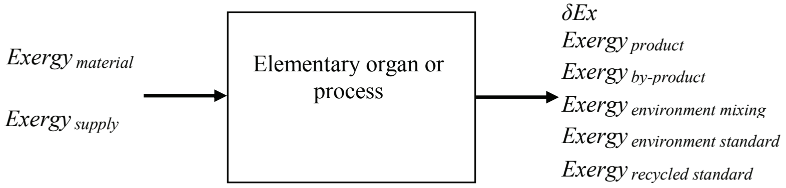


Figure 2: Types of exergy inputs and outputs in an elementary organ or process

The inputs of the process can be represented by the exergy of raw materials (*Exergy* $_{material}$) and the exergy supply (*Exergy* $_{supply}$). The outputs are represented by the exergy of the desired products and by-products (*Exergy* $_{products}$ and *Exergy* $_{by\text{-}products}$), exergy rejections to the environment computed via the exergy of mixing formula (*Exergy* $_{environment\ mixing}$), exergy rejections to the environment computed via the standard chemical exergy formula (*Exergy* $_{environment\ Standard}$), the flow of exergy of waste not directly rejected in the environment (*Exergy* $_{recycled\ Standard}$) and the exergy loss (δEx) due to irreversibility.

4.2 Material and resource consumption numbers (thermodynamic metrics)

The *Primary Exergy Conversion Efficiency* (PECE) is represented by the ratio of the sum of the useful output to the sum of the inputs that occurred to produce it. A high number represents a high efficiency in the overall management of exergy:

$$\prod PECE = \frac{Ex_{product} + Ex_{by-product}}{Ex_{material} + Ex_{supply}} \tag{5}$$

The *Material and Resource Consumption Efficiency* (MRCE) is represented by the ratio of the sum of the output, except the exergy loss, to the sum of inputs, except the recycled by-products. A product that has a high efficiency in its material and resource use will have a high Π_{MRCE} number:

$$\prod MRCE = \frac{Ex_{product} + Ex_{env-standard}}{Ex_{material} + Ex_{supply} - Ex_{recy-standard} - Ex_{by-product}} \tag{6}$$

4.3 Environmental impact number (environmental metric)

The *Environmental Impact Efficiency* (EIE) is represented by the ratio of the ratio of exergy of mixing to the exergetic inputs. As the exergy of mixing represents pollution, a high Π_{EIE} number signifies a high environmental impact:

$$\prod EIE = \frac{Ex_{env-mixing}}{Ex_{material} + Ex_{supply} - Ex_{recy-standard} - Ex_{by-product}} \tag{7}$$

5 CASE STUDY

5.1 Presentation

The case study is performed on two possible systems from a project in the early design phase: the plastic cover of a reconfigurable sand casting mould.

The first system, referred to as *System 1*, is made up of three parts:

- Plastic film – preformed, cut out from a large sheet, volume: 7.987×10^{-6} m^3
- Aluminium nest (top part) – 45g, machined
- Aluminium nest (bottom part) – 151g, machined
-

The aluminium nest is machined from two aluminium plates with the following dimensions:

- 120mm*120mm*5mm - 195g
- 120mm*120mm*20mm - 780g

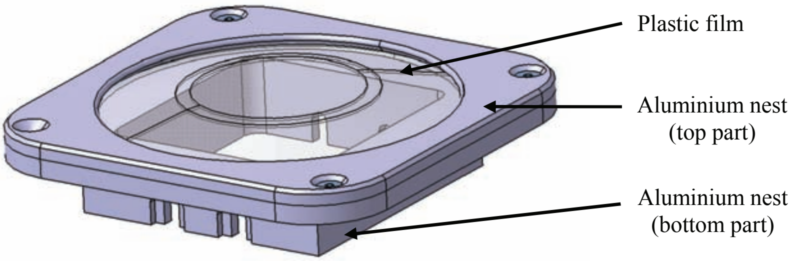


Figure 3: System 1

The second system, referred to as *System 2*, is made up of four parts:

- Plastic film – preformed, cut out from a large sheet, volume: $9{,}4*10^{-6}m^3$
- Rubber join – cut-out from a large sheet, volume: $2.265*10^{-6}m^3$
- Aluminium nest (top part) – 40g, machined
- Aluminium nest (bottom part) – 398g, machined

The aluminium nest is machined from two aluminium plates with the following dimensions:

- 120mm*120mm*6mm - 234g
- 120mm*120mm*22mm - 975g

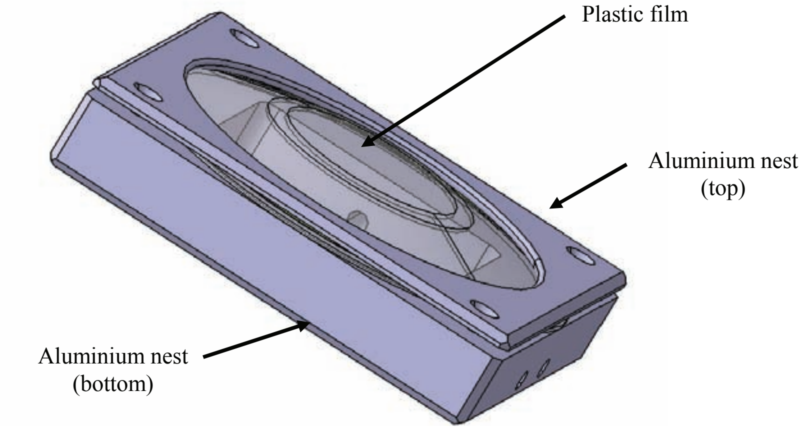


Figure 4: System 2

The machine used for all the aluminium parts is considered to a 15kW milling machine. The times for the milling are as follows:

Table 1: milling times for the aluminium parts

	Weight of raw part (g)	***Total scrap (g)***	***Machining time (s)***
System 1: top part	195	150	300
System 1: bottom part	780	629	1258
System 2: top part	234	194	388
System 2: bottom part	975	577	1154

The goal of the study is to assess the exergetic impact of the two systems using both the CExD LCA and exergetic approach.

5.2 Definition of boundaries

To ensure the comparability of the two studies, the boundaries are thoroughly examined.

The original designs for both System 1 and System 2 included four screws to hold the two parts of the aluminium nests together. In order to limit the amount of materials used and therefore simplify the study, we have chosen to disregard the presence of the screws. Indeed, the four same screws would be used in both systems and would be commercially bought.

The machining process that is used to make the aluminium nests is considered to have a perfect cooling liquid closed loop. The cooling liquid is recycled in its entirety in other milling processes. The material being aluminium, the machining can be done without cooling liquid if the cutting speed is kept low. This paper does not discuss the possibility of other production processes. For an exergetic comparison between a machining process and a process involving casting and milling, refer to [5].

One of the limitations in this study is the description of the materials used. The aluminium alloy used for the making of the parts is considered to be a standard general purpose alloy Al 98.7% Mg 0.6% Si 0.7%. Indeed, the parts discussed in this article are part of a project in development and are made using materials easily accessible and milled. To make the two studies comparable, the data used for the aluminium and steel parts are those provided by the eco-invent databases in SimaPro.

Moreover, the composition of the plastic film and rubber joint posed a problem. We make the hypothesis in the exergetic study that both are made from vulcanized rubber. Indeed the compositions of latex balloons and rubber joints are not easily found as the companies producing them prefer to keep them secret. The SimaPro study uses *Synthetic Rubber, at plant* as it is present in the ecoinvent database. Its composition is not given in the program and therefore cannot be easily used for the exergetic study.

The exergy of the assembly of the parts is not included in this study. The data for the energy necessary for the milling machine is based, for both approaches, on the data in the ecoinvent database for medium voltage energy produced in Finland.

5.3 Exergy LCA applied to the object

5.3.1 Modeling and inventory analysis

The first step of an LCA study is to make an inventory of the parts present in the systems. The inventory for System 1 is represented below in Figure 5. The second system's inventory includes a second part of synthetic rubber.

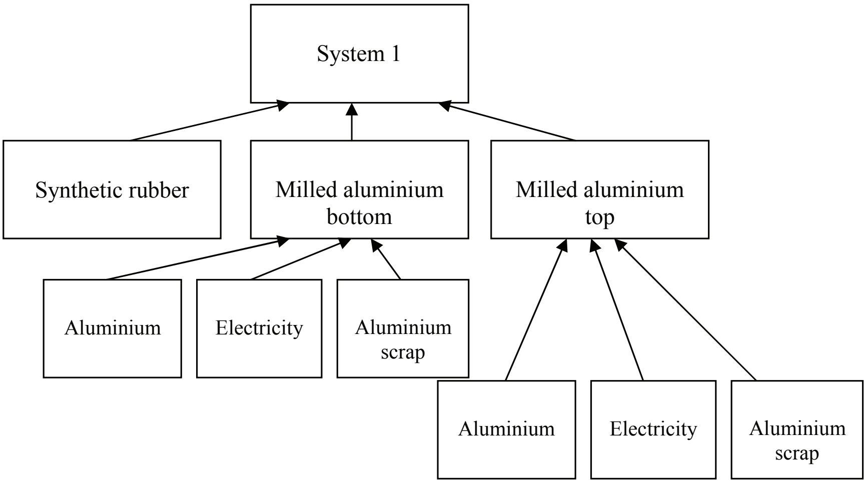


Figure 5: Model of System 1

5.3.2 Impact assessment

The two systems were compared using the CExD indicator. This method evaluates the amount of exergy loss in each category mentioned in the legend of Figure 6.

Table 2 contains the explicit values of the different exergetical impacts. All the categories but the potential exergy are more important for System 1. The most important exergetic impact is deemed to be the water exergy. As stated in [8], the exergy of water contributes on average to 8% of the total exergy demand but, in certain cases, this amount can increase to over 90%. In our scenario, the contribution is of around 94% for both systems. The water importance is due in this case to the important amount of water used in the processing of bauxite ore.

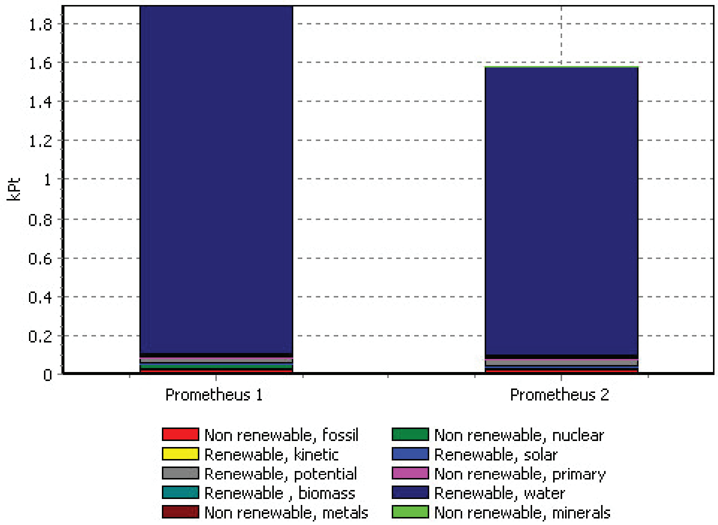
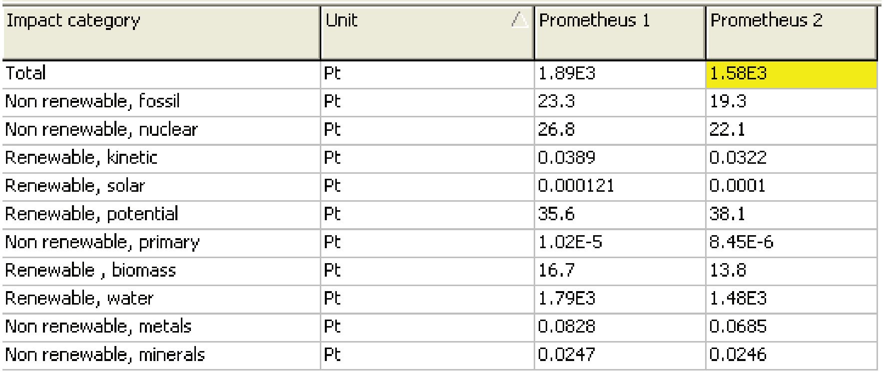


Figure 6: Comparison of System 1 ("Prometheus 1") and System 2 ("Prometheus 2")

Table 2:CExD comparison scores



Impact category	Unit	Prometheus 1	Prometheus 2
Total	Pt	1.89E3	1.58E3
Non renewable, fossil	Pt	23.3	19.3
Non renewable, nuclear	Pt	26.8	22.1
Renewable, kinetic	Pt	0.0389	0.0322
Renewable, solar	Pt	0.000121	0.0001
Renewable, potential	Pt	35.6	38.1
Non renewable, primary	Pt	1.02E-5	8.45E-6
Renewable , biomass	Pt	16.7	13.8
Renewable, water	Pt	1.79E3	1.48E3
Non renewable, metals	Pt	0.0828	0.0685
Non renewable, minerals	Pt	0.0247	0.0246

5.4 Dimensionless Π numbers applied to the object

5.4.1 Modeling and inventory analysis

The plastic film and rubber joint are represented with vulcanized rubber and the aluminium parts are made from an alloy containing Al 98.7% Mg 0.6% Si 0.7%. The density of the rubber is that of an average manufactured rubber, 1522 kg/m^3 [20].

Table 3 contains the data necessary to compute the standard chemical exergy [9]:

Table 3: Molecular mass and standard chemical exergy of single elements

Substance	***Molecular Mass (M)***	***Standard chemical exergy b^0_{ch}, kJ/mol***
Al	26.9815	888.4
Mg	24.312	633.8
Si	28.086	854.6
CH2	14.026	651.46
CH=	13.018	569.95
C=	12.01	473.02
CH3	15.034	752.03

CH-	13.01	549.91
C-	12.01	436.03
S	32.06	642.32

The different exergies indicated in Figure 8 were calculated using the standard chemical exergies in Table 3, the milling times indicated in Table 1 as well as the amounts of CO_2 rejected into the atmosphere as indicated in the ecoinvent database.

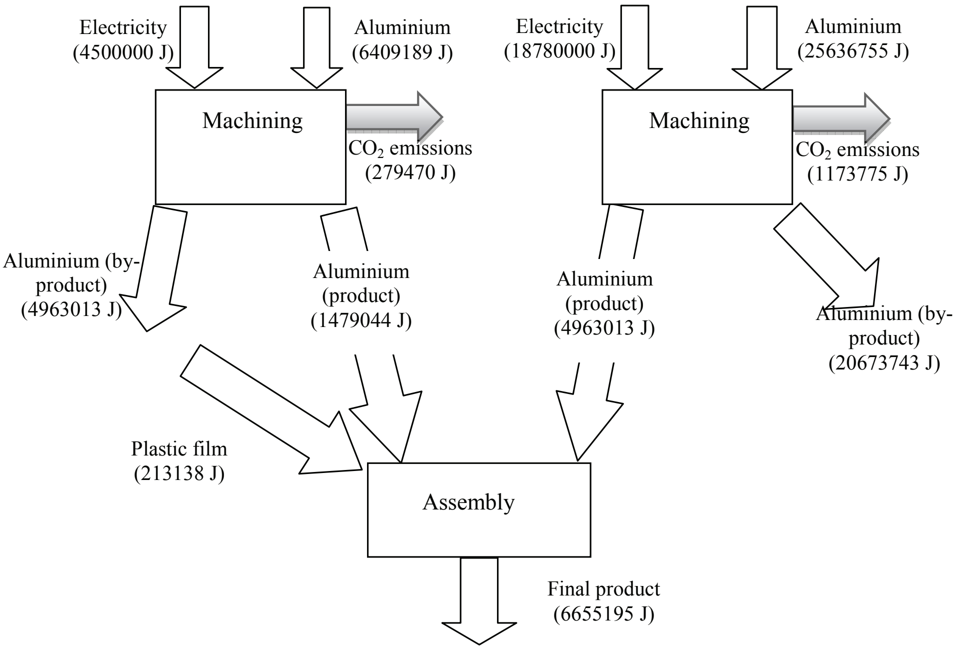


Figure 8: Model of System 1

5.4.2. Impact assessment

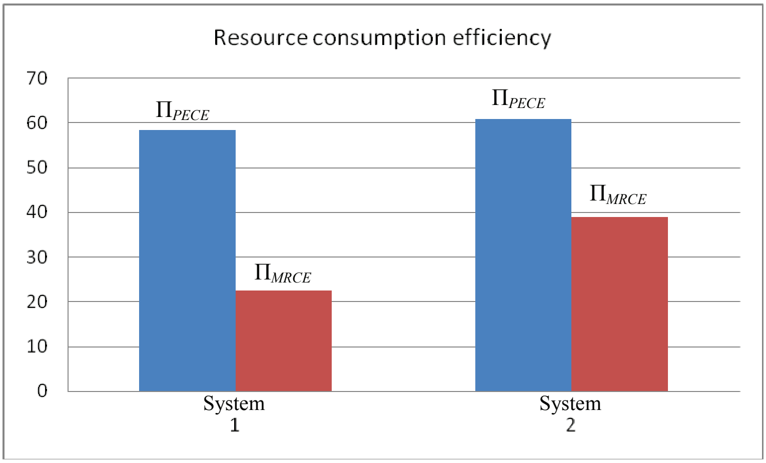


Figure 9: Resource impact assessment

As mentioned in Section 4.3. the Π_{PECE} and Π_{MRCE} numbers represent efficiency. Therefore they should be analysed in the following manner: "*the higher the better*". Therefore System 2 is more efficient from a resource consumption perspective than System 1.

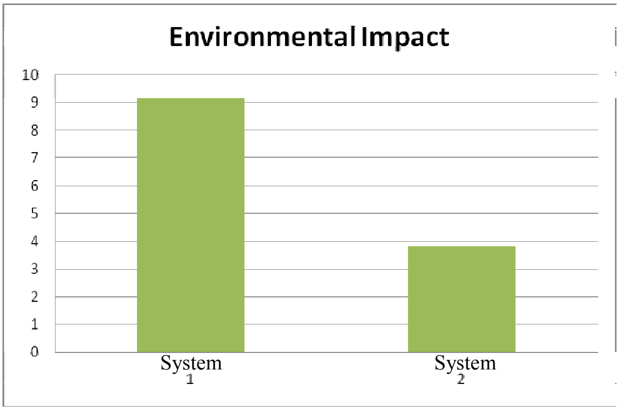


Figure 10: Environmental impact assessment

Π_{EIE} takes into account the exergy of mixing of different emissions of substances produced along with the final product but which are then rejected into the environment. In this study, the rejections considered are those of CO_2 emitted during energy production. System 2 presents less environmental impacts for CO_2 emissions.

6 COMPARISON

The two approaches above yield concordant results. Indeed, the CExD method points out that System 2 leads to a smaller exergy removal from nature to create it than System 1 and the Π number method shows that System 2 uses resources more efficiently than System 1. The two methods cannot be compared number to number because the logic behind them is different.

The first method assessed in this article, the application of the CExD indicator to the ecoinvent database is based on the computation of the total exergy removal from nature to provide a product [8]. The exergy removal measured with the CExD indicator is categorized into eight resource categories fossil, nuclear, hydropower, biomass, other renewables, water, minerals and metal. As it is known since Lavoisier, energy and matter used in society cannot be destroyed but only transformed. The usable energy and usable matter consumed are eventually depleted. The CExD indicator measures the quality of the energy and matter demand, it focuses on the amount of exergy removed from nature and the quality of this exergy. The approach pushes users to optimize the usage of resources of high quality, especially water, but *not to measure the scarcity of resources nor the environmental impact nor the impact of the disposal phase of end-of-life products or elements in the environment*. These three aspects represent in our perspective three rather important drawbacks of the approach that do not take into account two fundamental aspects of exergy, its ability to “close the loop” of life cycle analysis and the possibility to compute exergy of mixing that can be considered a manner of solving the two last issues.

The second approach combining an exergetic approach and Π numbers offers, in our viewpoint, a solution to the three limitations of the CExD indicator. This is due, for the two last points, to the fact that our calculations take into account the exergy of mixing. In addition, the scarcity of resources can be considered by providing the exergy of mixing (Equation (4)) with a reference activity (γ_i^0) in the appropriate environment (sea, earth crust or atmosphere) adapted to the concentration of the local environment.

The combined exergetic and Π numbers approach is based on a different philosophy than CExD as it considers that the environment has a certain auto-regenerating capability (for at least some resources). Another difference in the vision of an environmentally friendly behaviour defended by this second approach is the possibility to release processed substances in the environment if they occur naturally in it. The only recommendation made by the authors is to release after reprocessing to ensure that the concentration level of the substance and its chemical form are similar to the local composition and reference activity of the environment. If a substance does not exist naturally in the environment, it should be reprocessed, if possible, into substances existing in the environment. The other alternatives are the destruction or the storage of the substance if no reprocessing solution exists. All these strategies derive logically from this second type of exergetic approach.

Nevertheless, the results of the two approaches are concordant but the scope of the second approach is broader. This is the key point of the analysis which tends to demonstrate once more that the exergy coupled with Π numbers approach provides coherent results.

7 CONCLUSION AND FUTURE WORK

The present article has presented further validation for the use of exergy coupled with dimensionless numbers to complete environmental assessments. The concepts of exergy and Π numbers provide a uniform metric for such evaluations. The concordance of the results obtained with the two approaches studied in this article is a step toward the complete validation of the exergetic and Π numbers approach in the early environmental evaluation assessment. While this study shows a case study of the application of exergy to an engineering problem, future work will include more complex scenarios and will not be limited to products or processes but will be extended to services.

The framework used in the exergetic and Π number study is based on existing information already published in books treating exergy. Moreover, the calculations of the Π numbers do not require many resources and therefore can be easily integrated into other software.

Future work will concentrate on the development of an environmentally oriented design tool for the early design phases. Multiple branches are currently being studied for a further evolution of the tool such as integration of value and decision theory. The final aim is to provide a tool which is light and can be incorporated into other design tools such as CAD software.

As presented above, this research is part of a larger project which will include multiple ontology layers mapped together using the simantics language. Each layer will represent a part of engineering design such as exergy, for environmental purposes, requirements, etc. More than an environmental evaluation tool, the idea is to create a model-based approach for the whole early engineering design process.

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