The strategic role of Life Cycle Assessment in the problem of material criticality and in development of Chromium-free substitute for stainless steel

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Abstract. Sustainable and on-going technological developments in the field of materials require the establishment of methods and tools for assessing, comparing environmental impacts and providing solutions to the problem of "resource criticality" by identifying a policy of an economic and ecological plan. Therefore, there is a clear need for prevention and provision of additional knowledge beyond the defined protocols to achieve the reduction of impacts. For this reason, Life Cycle Assessment (LCA) has been developed as a scientific technique that systematically assesses and evaluates the environmental impacts associated with all stages of a product's life. In this work, LCA was applied in a part of a highly innovative process of production of advanced Iron-Aluminum (Fe-Al) based intermetallics. LCA role is particularly crucial, since the produced intermetallics are bound to substitute stainless steel, in specific applications, providing solution in the problem of Cr and Ni; as a result, the environmental burdens and impacts, as well as application of alternative solutions to minimize them, will decide if such an innovative, from the technical point of view, approach is also applicable/sustainable in large scale.

1 Introduction

The environmental sustainability and the technological development of all materials are undoubtedly continuously resurfacing issues. At the same time, due to the increasing technological advances with requirement of new materials, that transform the everyday life with increasing socio-economic benefits, the necessity of treatment of the materials for the effects from the cessation of supply and demand, Life Cycle Assessment (LCA) of materials, safety assessment and criticality of resources have emerged. [1]

Raw materials are the basis for the synthesis and production of the vast number of products and applications used in everyday life. Rapid technological innovation and the accelerated development of emerging economies have led to the establishment of a list of Critical Raw Materials (CRMs) at European level, in order to address the concern of securing the uninterrupted function of the European industry. However, there is a concern about CRMs. Several alternatives are under consideration for their substitution. Replacement may be made from alloys, super alloys and intermetallic compounds containing Chromium (Cr), Nickel (Ni), Aluminum (Al), Iron (Fe), Molybdenum (Mo) and Vanadium (V). Intermetallics can be a promising choice of CRM-containing materials (such as stainless steel) replacement. This is in line with the European scientific and strategic implementation plan with a view to assuring a sustainable supply and the secure, strong consolidation of the European Union in the world of materials.

Fe-Al based intermetallics are not used in large scale applications. Despite the fact that they have superior resistance to corrosion and erosion, lower density and higher hardness, melting point, with respect to stainless steel, they are relatively brittle at intermediate and low temperatures, while they have poor machinability. The intense study on intermetallics in the 50's and 60's did not manage to solve the above shortcomings. Currently, a new production method is being intensively studied, within a H2020 funded project named EQUINOX. The EQUINOX approach is based on the control of intermetallics' microstructure; more specifically, on the grain refinement of the end products, which will provide increased ductility and improved machinability.

Responding to these critical issues, LCA contributes to the minimization of the uncertainty of technological assessment, by identifying and calculating potential material concern. LCA is a method, which evaluates and compares the environmental impact of human activities at all stages of a product's life. The purpose of LCA is to initially identify all environmental impacts, to minimize them, with the study of these innovative and improved materials that, due to important advantages in the field of Green Public Procurement (GPP), will have the key role as substitutes. In addition, the safe production and use of products is achieved, as well as the identification of material substitution opportunities with a view to limiting the criticalness of raw materials availability and consequently CRMs availability. [6] Moreover, with the internationally standardized LCA methodology, the competitiveness of all sectors is enhanced, leading to a radical innovation in the world of materials, with the interaction of companies, industry, education and research. In addition, it gives the possibility of entry of the intermetallic compounds, which, as substitutes, will help with sustainable economic production and environmental balances. In this way, through the well-established LCA tool, a complete impact of a product is finally obtained along with a detailed record of the resources allocated to the supply of goods and services and the energy and environmental footprint of the overall process. [1]

In the present work through the LCA technique and in particular using software SimaPro© and method IMPACT 2002+, beyond the environmental impact assessment and pressures, a great innovation benefit is achieved, namely, the substitution of CRMs from intermetallic compounds.

This substitution is an alternative for improving material criticality, reducing consumption of commodities and resources and obtaining a clear reduction of dependence of the European market from CRMs in processes of extreme conditions, since Fe-Al intermetallic compounds ensure improved properties, risk reduction across all sectors and an energy-efficient profile.

In conclusion, all these actions incorporate the strategic role of the LCA tool through which results and analysis are important for decision-making at an industrial, economic and political level. Finally, an additional indication of the necessity of the LCA is the direct relation to the risk assessment, its calculation as well as its proper management. [5]

2 State of the Art: Structure and methodology of LCA tool

LCA has been developed as a scientific technique that systematically assesses the environmental impacts associated with all stages of a product's life. In particular, life stages are the extraction of raw materials, processing, distribution, use, disposal, transport and recycling (Fig.1). The numerous impacts occurring at different stages of life cycle include emissions to the environment, resource consumption and other burdens incurred throughout the life processes and stages. All loads that play a separate role contribute to a wide range of Midpoint categories as well as to General damage categories, which are displayed in the Fig. 3. [1],[6]

Fig. 1. Schematic representation of a generic life cycle of a product (the arrows represent material, energy flows and information flows) [1]

LCA methods are increasingly being applied to ensure and enhance the supply of funds, which is key to political and business concerns. Also, this scientific technique favors balancing in the material sector, the existence of a material input / output balance for the directly related industries, since the criticality of some materials reduces access to raw materials. Additionally, the LCA process is based on four methodological elements that are closely connected to each other, as there is continuous interaction to produce a complete stud. [6]

The methodological elements that constitute the framework of the scientific tool are: Goal and Scope Definition, Life Cycle Inventory Analysis (LCI), Life Cycle Impact Assessment (LCIA) and Life Cycle Interpretation. (Fig.2)

Fig. 2. Illustration of LCA phases and applications (based on ISO 14040:2006)

Prior to the detailed description of the methodological elements, it is necessary to bring the ISO (International Organization for Standardization) standards that define the proper functioning of the LCA.

The ISO 14040 standard defines an LCA as a compilation and evaluation of the inputs and outputs and the potential environmental impacts of a product system through its life cycle. In this definition, it is clear that impact assessment plays an integral part in a LCA. The framework of these standardization authorities, which is responsible for the methodology, is concerned with defining the goal and scope of the LCA, the LCI phase, the LCIA phase, the Life Cycle Interpretation phase, reporting and critical review of the LCA, limitations of the LCA, the relationship between the LCA phases, and conditions for use of value choices and optional elements.

Specifically, ISO 14040:2006 covers LCA LCI studies. It does not describe the LCA technique in detail, nor does it specify methodologies for the individual phases of the LCA. [4]

2.1 Goal and Scope Definition

Goal and Scope are cardinal constituents of LCA methodology. The correct definition of these terms from the outset will lead to a good environmental management and will help in obtaining the necessary information and strategic decisions since they can have a significant impact on the results of the LCA analysis.

However, in order to achieve this goal, it is necessary that the objective and the scope of application are clearly determined at the beginning of the process study, at the design and development stage of the material. [1]

In addition, one of the most important actions that will lead to an integrated research environmental approach is to fully understand the boundaries of the system being studied. At the same time, there is a full list of inputs / outputs of materials through which the efficiency of processes, the energy footprint, the emissions produced and the options / processes at the end of the life cycle of the material will be perceived.

2.2 Life Cycle Inventory analysis and Data Collection

Analysis of the LCI or life cycle review is one of the main goals of this work. It is a detailed methodology for recording and estimating the consumption of resources, quantities of waste and emissions flows within and outside the product system from the time of extraction of the raw materials to their recovery and recovery of energy. Initially, in a production process to achieve quantification of materials and energy flows, not only quantitative data but also qualitative inputs, collection of inputs and outputs related to the operation or products generated by the process should be collected. [7]

The LCI phase, in other words, the analysis of environmental "interventions" is based on the collection of data for each process of a product system. Collection of data is an extremely detailed and time-consuming work, but it is an integral part of the implementation of the LCA. The data is the total input / output flows of the process. Specifically, raw materials, chemical products that are part of the production process, emissions, supply and consumption energy, means of transport, waste treatment, recycling scenario. All data must be quantified and the correct unit of measurement given. Many of the data used are available in the SimaPro software database but it is not always the case. In the case of lack of appropriate data, user is obliged to define and insert the missing data in the database by defining a standard quantity of it. [1]

2.3 Life Cycle Impact Assessment

At the stage of life cycle assessment, an assessment of the potential effects of the life cycle through the data collected at the inventory stage is carried out. Potential impacts can be replicated at the "midpoint" or "endpoint" level. (Fig.3) The "endpoint" marks the end of the cause-to-cause link of the overall production process. [6] Furthermore, the assessment of environmental indicators based on actual, verified, qualitative and quantitative data reflects real chains of industrial processes. In addition, the "endpoints" are much more tangible and accessible for the presentation of the outcome of a process and for understanding the impact on human health, ecosystem, climate and resources. On the contrary, "midpoint" is more abstract since it concerns, for example, effects on the potential of photochemical ozone, with a lower level of uncertainty. [6]

Fig. 3. Midpoint-class categories and estimations for the impact on the general categories of damage provided by LCA

2.4 Life Cycle Interpretation

In order to complete the process, it is necessary to interpret all stages of the life cycle. The performance and interpretation of the results through the interaction of the three previous stages involves the identification of important issues in which the LCA method will provide solutions, an assessment of the balance among human, ecosystem and social environment. In addition, produced results are related with the comparison of materials and categories of impacts as well as, in the present work, with the evaluation and the proposal as a salvage solution to substitute CRMs-containing stainless steel with CRMs-free intermetallic Fe-Al compounds. All these actions aim to produce improved and more environmentally friendly materials, to minimize the depletion of resources and to create new prospects and opportunities for materials, which will help to increase European sustainability, economy, industry, research progress and innovation.

3 LCA for the efficient management of CRMs and substitution of stainless steel in intermetallic compounds

According to the European Commission decision of 2014 on CRMs [2], Cr was included in the list of critical raw materials. However, according to the decision made in 2017 [3], Cr was not found on the list. However, this does not mean that there is a complete lack of criticality or that it will not be listed again as a CRM. Cr metal is under consideration for substitution, because the European industry requests to produce huge quantities of stainless steel, but the European world of materials can't support for the necessary quantities of Cr. In 2017, the European Commission identified 27 critical raw materials at European level. [3] These Raw Materials are characterized as critical, based on two parameters: (a) their economic importance for the production base of Europe and (b) their supply risk not necessarily because of their scarcity in the Earth's crust but also because of their concentration in countries with questionable governance performance and trade aspect, from the European point of view. The high demand of raw materials led to the creation of a group of critical raw materials for which substitutes are needed in order to encounter the shortage and the lack of supply.

The implementation of LCA has led to an effective management of CRMs and to a guiding policy of finding opportunities for raw material innovation and CRMs, respectively. By applying the LCA method, inventory analysis, depletion potential, material yield, open the pathway to minimize the use of CRMs and to facilitate their substitution by the Fe-Al structural elements of intermetallic compounds. This research work focuses on the substitution study of stainless steel parts containing significant quantities of CRMs, mainly Cr and Ni and, to a less extent, Mo and V, widely used in many industrial applications, especially in extreme conditions for corrosion and wear resistance. The research guidelines have solved the problem of the depletion of raw materials by using Fe-Al

intermetallic compounds which have many attractive properties such as high melting point, good thermal conductivity, high resistance to corrosion and wear, and controlled industrial impact, as described at the Introduction section. Moreover, Fe-Al intermetallic compounds are characterized by low production costs, as opposed to the critical material chromium. Finally, one more positive feature of Fe-Al intermetallic compounds is the substitution of Cr-Ni based stainless steel parts from Fe-Al. With this process, CRMs are relieved of "risk of death" as there will be continuous abundance of Fe and Al in a process - chain.

4 Modeling of LCA tool, manufacturing procedure and interpretation of results

The LCA study of the process was “Machining Fe₃Al with Hard Metal (HM) tools” performed with the SimaPro software and specifically using the Ecoinvent.v.3.3 database and the IMPACT 2002+ method. [4] Process under study is based on standard procedure of Computer Numerical Control (CNC) technologies (milling, drilling, polishing, grinding, lathes, cutting). In particular, an intermetallic (Fe-Al) preform is treated (metal cutting machining) with a CNC procedure for the production of the bumper end product. Table1 shows the corresponding life cycle inventory data.

Table 1. Life cycle inventory collected data and selection from SimaPro database. the right column includes optimised figures based on our experience and relative literature

Input given	Selection from SimaPro database
Machining time of 1 kg Fe ₃ Al with HM tools	0.1 kgy
Water 3l/h	0.003 m3 Water cooling
Concentrated CURTIS High-speed cut suspension 2450,011/h	0.0098 kg _l ubricating oil
Electricity consumption:40kWh per machine	40 kWh electricity mix
Metal waste: HM tool 0.1 kg	0.1 kg reinforcing steel
Metal waste: Fe ₃ Al (cuttings) 0.1 kg	60 g iron pellet & 40 g aluminum, primary, smelt
Truck for transport of bumper end product <1000 km	0.9 tkm small lorry transport
Train for transport of building machines >1000 km	1.1 tkm transport, train, diesel powered

The inventory was established with the cooperation of Elastotec GmbH company that has a strong background on CNC technologies, which manufactures its own products with a strong focus on process industry. Because of the huge volume of data collected, SimaPro has been designed to perform LCA calculations in an automated way and with the use of specialized algorithms. [4] Through the software, the effects of the manufacturing process of products and services at all stages of their life in accordance with ISO rules are presented in the form of charts. (Fig.4) First of all, in order for the LCA study to be carried out properly, it is necessary, besides defining the system boundaries, to clarify the function of the system and the functional unit. The function of the system we are studying is the “Machining Fe₃Al with HM tools”. The functional unit defines the unit by which the environmental impacts of the process are described and calculated. In this case the functional unit is 1 hour of machining Fe₃Al with HM tools. It is necessary for the calculations, input / output data, raw materials, energy, sources, wastes to be quantified and defined their measuring units. (ISO 14044:2006) [6]

The reference flows, the inflows and the outflows and the impacts that arise through each functional unit, are calculated by a well-established system. The system is not defined only by sums of inflows / outflows, but also by connections and interactions between them. This connection wants to emphasize that the modeling of the system is a holistic approach with a dynamic character. [6],[7]

After the collection of the necessary data from all the life stages of the material, the assessment and the calculation of the effects are followed. This is done through the categorization of emissions into different impact categories, the characterization of midpoint impacts and the characterization of the end point. It should be stressed that inventories recorded by such influences should be categorized at an intermediate level, the so-called midpoint category. For each midpoint category, a midpoint marker is defined. All inventory flows are multiplied by a characterization factor. In this way, the impact of the overall process in the midpoint category is quantified and characterized. Then each midpoint category is branched into general damage categories (endpoint categories) which are characterized by a damage indicator or else by an end point indicator. So, with this way there is a reduction from the midpoint category to endpoint category. [6],[7]

Finally, with the introduction of process data into the software database and the automatic calculation of the damage indicators and the algorithms, the following charts are presented. These charts (Fig.4) show the overall behavior and effects of the process both in the midpoint categories and in the endpoint categories.

It is evident from the results of the charts (Fig.4) that the production stage is the one with the highest burden. The results in the midpoint categories are more accurate and more detailed in relation to the results in the endpoint categories that are more tangible. In the midpoint categories it is observed that the electricity consumption is responsible for all the negative effects in all fields. The high burden is due to the mechanical aggressive behavior of the machining infrastructure. Also, there is low impact from concentrated CURTIS High-speed245 (lubricating oil) cut suspensions and iron pellet.

Finally, there is a high positive effect from HM tools (reinforcing steel) and Fe₃Al cuttings which, however, occur as waste from the process and have the advantage of high recycling potential. Recycling is of great importance because it minimizes charges in all fields.

In the endpoint categories the extremely negative impact of electricity in all categories is identified. This effect is pretty reasonable for the process, machining Fe₃Al with HM tools.

In addition, in the endpoint categories, a positive influence of the metal wastes is observed. The positive effect from HM tools and Fe₃Al cuttings is better represented in the Table 1. In this table there is quantified impact in Eco-Point Units ($\times 10^{-5}$) on endpoint categories. The positive effect is expressed by the negative values.

Fig. 4. Analyzing 1kgy 'machining time of 1 kg Fe₃Al with HM tools'. Method: IMPACT 2002+ /Midpoint categories (left)/Endpoint categories (right)

Table 2. Quantified impact in Eco-Point Units ($\times 10^{-5}$) on Endpoint categories

		Impact in Eco-Point Units ($\times 10^{-5}$)			
		Human Health	Ecosystem Quality	Climate Change	Resources
Process stage	Machining time of 1 kg Fe ₃ Al with HM tools	0.0	0.0	0.0	0.0
	Concentrated CURTIS High-speed245,cut suspension	1.65	0.289	1.11	5.35
	Electricity consumption	640.0	20	2680	2.81
	Truck for transport	20.0	42.6	10	1.0
	Train for transport	0.0	0.0	0.0	0.0
	Concentrated CURTIS High-speed245, cut suspension	-1.65	-2.89	-1.11	-5.35
	Metal waste HM tool	0.0	-4.27	0.0	0.0
	Metal waste Fe ₃ Al (Fe cuttings)	-3.29	-41.2	-68	-69.5
	Metal waste Fe ₃ Al (Al cuttings)	0.0	0.0	0.0	0.0

5 Concluding observations and outlooks

The aim is to discuss the advantages and limitations of the LCA process as well as to propose alternative solutions to minimize the burden. The environmental impacts of the process "Machining Fe₃Al with HM tools" as well as the "focal" environmental burden were identified and assessed. Also, possible improvements were made by taking into account the life cycle conditions of each activity.

The obtained results underline that the main negative impact on all categories, midpoint and endpoint, and on all sub-fields is due to electricity consumption. One way of minimizing this negative impact is to replace electricity source with another source that includes alternative forms of energy (energy derived from biomass, solar energy, wind energy) and minimizes the use of fossil fuels. However, apart from the negative impact, there is also a positive effect which contributes to the solution of criticality of materials. By analyzing the LCA of Fe₃Al compounds, it was observed that the waste resulting from the process can be recycled. Metal waste is composed of Fe₃Al cuttings and HM tool (reinforcing steel) cuttings consisting of Fe. Recycling is a salvage solution in the world of materials, making intermetallic Fe-Al compounds capable to be used as substitutes for CRMs, namely Cr-Ni in stainless steel parts. Apart from the good mechanical properties of the intermetallic compounds that make them suitable substitutes, recycled materials can re-enter the system and be re-used. There is, therefore, a cycle of continuous renewal of materials. In addition, recycling of intermodal compounds will help to achieve environmental, economic and human balances, investment decisions and market and technology enhancement.

A key challenge for industries is to be able to trust and assimilate the data produced and the conclusions drawn from the LCA method in a way that is useful for business management, macroeconomic decisions and effective policies of the products. An additional prospect is to link LCA to the Life Cycle Cost (LCC) analysis. This connection will serve as a pillar for sustainable development, will give "breathing" to industries realizing more efficient management and costing of processes.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Grant Agreement No. 689510 Furthermore, we thank Elastotec GmbH for collaborating and providing the data through which the Life Cycle Analysis was done.

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