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Excel tool to assess the environmental impact of steels based on the composition

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Abstract

The communication shows the simulation tool developed to calculate the environmental impact of steels based on their composition. The tool is based on the modeling of the Life Cycle Inventory of steels, and only requires the composition data of the steel as input data. This modeling of the systems allows to quantify the content of critical raw materials, which, despite not being a regulatory requirement, may constitute a good practice as a better use of the available resources.

The different blocks of the tool are detailed in this communication: input data, calculation methodology and the results display block. At the same time, a case study is shown, where the environmental impact of three steels are used in the manufacture of metal components of LED luminaires has been simulated. The results have been compared with those obtained from the models provided by EcoInvent, in order to represent the relevance of perform a more accurate simulation of environmental impact based on the composition. Likewise, the content of critical raw materials of the three steels analyzed has also been obtained.

Keywords: Life Cycle Assessment; Simulation tool; Critical Raw Material; Environmental Impact; Steel

1. Introduction

Steel is the most widely used metal in the industry. Its versatility and good mechanical properties make its applications numerous. It is known that steel is essential to current technologies and economic activities (Wang et al., 2020). And, in addition, with rapid urbanization and industrialization, the steel demand has increased over the last several decades (Sun et al., 2020).

A current challenge for companies and economies worldwide is to develop more sustainable and environmentally friendly economic systems (Chen & Huang, 2019) (Fernández-Viñé et al., 2013). The use of good practices and efficient management of resources is an intended aim by companies and government institutions. That happens due to different factors: a demanding environmental legislation, cost savings (thanks to efficient technologies or intelligent resource management) or to obtain a competitive advantage in the market (Borchardt et al., 2011).

The circular economy plays a fundamental role in the European Union. Since 2015, it has promoted a transition of its economy towards this production model (European Commission, 2015) and its purpose continues with the Green Deal adopted in 2020 (European Commission, 2019) (European Commission, 2020a). The main actions leading towards a Circular Economy are related to value capture: maintain the value of products, materials, and resources for as long as possible within the economy (Ranta et al., 2018).

In the last three decades, ecodesign has been adopted by many companies and engineers (Brambila-Macias & Sakao, 2021). It is also part of the legislative offer of the European Union (Directive 2009/125/EC) (Directive 2011/65/EU) (Regulation (EC) No 1907/2006). This trend of thought assesses all the environmental impact which occur in every phase of the product's life. Ultimately, it is about simultaneously integrating economic, functional and environmental aspects, with the aim of promoting sustainable development (Margallo et al., 2021).

This assessment takes place in the first phase of product development and allows taking corrective actions to reduce the adverse impacts of products on the environment (Ribeiro et al., 2013).

To assess the environmental performance of products and production systems, numerous tools have been developed with two main approaches: scientific and industrial. Among them, the Life Cycle Assessment stands out. This tool proposes to model the referenced system, identifying and quantifying all the inputs (matter or energy) and all the outputs (emissions, effluents, and solid waste) to the environment, throughout the complete life cycle. It considers all the existing stages: the extraction and processing of raw materials, production, transport and distribution, use, and the final disposal or recycling. In this way, it is possible to evaluate the environmental loads associated with a product. LCA has been applied to a wide range of sectors, processes and products (Heidari et al., 2020) (García-Alcaraz et al., 2020) (Farjana et al., 2019) (Martínez et al., 2015) (Tsiropoulos et al., 2015) (Jiménez et al., 2014) (Cellura et al., 2012).

Depending on the LCA, executing an LCA requires extensive data mining which is time-consuming and expensive. Therefore, the use of databases is greatly relevant. These databases parametrize a specific material, process and transport based on the aspects that generate environmental loads. This method models the system according to environmental parameters and allows to simulate of the environmental impact.

Due to the increasing use of LCA, numerous databases have been developed. These include the necessary information to characterize the inputs of matter and energy, as well as the emissions to the environment from materials and processes.

Modelling an LCA using databases is a method widely accepted by the scientific community. Nevertheless, can incur in approximations that hinder decision-making in the design or redesign of a product (Kalverkamp et al., 2020). It is, therefore, an iterative process to obtain an increasingly accurate result of the environmental impact of the products. Therefore, it may be interesting to carry out a particularization of the databases with the aim of obtaining a more accurate environmental impact calculation. This particularization is usually performed on materials or production processes.

The EcoInvent database (Wiedema et al., 2013) stands out for being one of the most complete ones and with a high quality, being the most widely used in the scientific field. However, in the specific case of steels, it only has three characterized types, corresponding to the categories included in the EN-10020 standard (AENOR, 2001), according to the amount of alloying elements present. According to the World Steel Association, currently, there are more than 3.500 types of steels in the market (*Worldsteel Association, 2021).* Therefore, considering the great variability of steel composition, the three datasets included in the ecoinvent database are considerably scarce.

The variability of the elements that make up a steel alloy not only determine its mechanical and physical properties (Kalpakjian et al., 2008) but also its total environmental impact. Previous works consider the importance of making a more accurate LCA modelling, considering the exact material composition (Gómez et al., 2015). In previous studies, a detailed calculation of the environmental impact depending on the composition has been carried out for aluminum alloys (Gómez et al., 2016) and magnesium alloys (García Gutiérrez et al., 2020). In both cases, the importance of this particularised calculation is revealed, with impact variations of up to 65% among different aluminum alloys and 29% among magnesium alloys, according to ReCiPe methodology. These studies also show the significant variations obtained between the composition-specific calculation and that obtained using EcoInvent databases. In other study about the alloys commonly used in marine construction (Kappenthuler & Seeger, 2021), a particularisation of the metal alloys is already made from EcoInvent datasets by adapting them to the desired alloy composition. This studies show that there is a research gap, and that the variations of the environmental impact of steel alloys depending on the composition should be analyzed.

This modelling provides the designer with more information on the environmental performance of the selected steel, allowing companies to opt for more sustainable options and make smart and efficient use of available resources.

Another important aspect is the efficient use of Critical Raw Materials (CRM). Since 2011, the European Union elaborates a material list considered relevant to the European industry. Economic importance and risk of supply are the two criteria used to classify these materials. Those materials that have simultaneously high economic importance and high supply risk are considered critical (European Commission, 2014). Many of these materials, could be associated with a high environmental impact. Nevertheless, this factor is not currently considered to assess the criticality of materials. To assess the CRM content in the design phase, can contribute to reduce their use and to highlight their link with economic, supply and environmental impacts (Ferro & Bonollo, 2019) (Kim et al., 2019).

2. Software development and LCA modelling implementation

Inventory of the steel production, depending on their composition. In this manner, it is possible to simulate the environmental impact. The tool has been developed with an Excel interface. Figure 1 shown the three differentiated blocks that establish the flow of the data in the Excel application: the input data, the methodology of calculation and the output data, which are explained in the following sections.

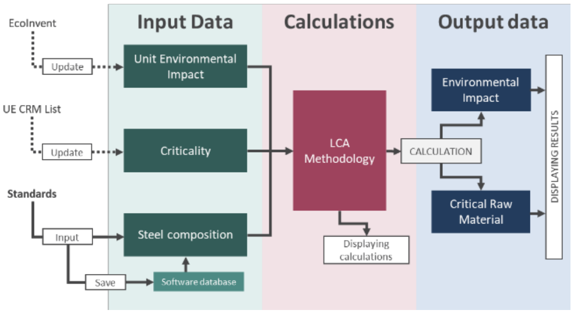


Figure 1. Flow of data in the developed tool

2.1. Input data and source of information

To model the Life Cycle Inventory of steel production, and then simulate the environmental impact, it was necessary to establish the following data:

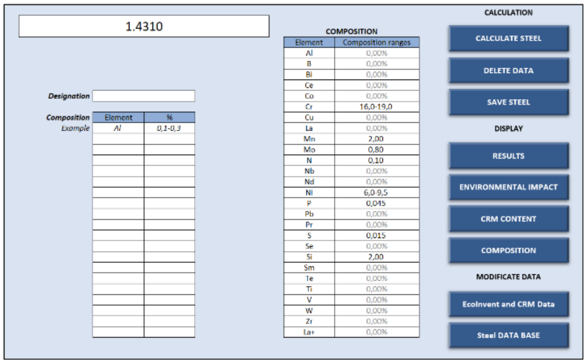
- Composition data of steels are the main information that the user must select. These data allow the system modelling and the environmental impact simulation.
- Environmental impact data of the different raw materials included in the alloy: alloying elements, base metals, and manufacturing resources.
- Criticality data of different alloying elements included in the steel alloy, and their classification as critical raw material or not.

It is noted that both unitary environmental impact and criticality values are not stable in time. Environmental impact results are subject to the updating of calculation methodologies of environmental impact. Similarly, criticality data are subject to market variations. Regarding CRM, the European Union study, update and publish this list every three years, to represent the market evolution. Criticality data were collected from the Critical Raw Material Report of the European Union, of which the last update was published in September 2020 (European Commission, 2020b). This report assigns values of both supply risk and economic importance to all the materials considered strategic for the European industry. And based on these values, classify them as critical or strategic.

Both dataset, environmental impact, and criticality of materials, have been incorporated in Excel application as a database, which can be updated according to the appearance of more recent data in an easy way.

Although all three blocks are needed to model the system, the only information required from the user is the material composition data. Steel standards are instrumental in classifying and specifying the chemical, mechanical and metallurgical properties of the different kinds of steel and ferrous alloys. These standards help guide metallurgical laboratories, manufacturers or end-users in the proper application of steel.

The composition data generally comes as composition ranges that can be input in the main screen of the Excel application, shown in Figure 2.



1.4310

Designation

Composition	Element	%
Example	Al	0,1-0,3

COMPOSITION

Element	Composition ranges
Al	0,00%
B	0,00%
Bi	0,00%
Ce	0,00%
Co	0,00%
Cr	16,0-19,0
Cu	0,00%
La	0,00%
Mn	2,00
Mo	0,80
N	0,10
Nb	0,00%
Nd	0,00%
Ni	6,0-9,5
P	0,045
Pb	0,00%
Pr	0,00%
S	0,015
Se	0,00%
Si	2,00
Sm	0,00%
Te	0,00%
Ti	0,00%
V	0,00%
W	0,00%
Zr	0,00%
La+	0,00%

Figure 2. Data entry screen

The Excel application includes a steel database, in which composition has been entered previously. In this way, if the steel is already available in the database, it can be selected from a drop-down list, and the composition will be shown.

2.2. Life Cycle Assessment Methodology

The simulation tool implements a calculation methodology based on a Life Cycle Assessment approach. Although explaining this methodology is not the object of this communication, certain aspects are explained in next subsections. The LCA has been developed following the stages stipulated in the international ISO 14040 (AENOR, 2006a) and ISO 14044 (AENOR, 2006b) standards that establish principles, framework, requirements and guidelines to perform an LCA.

2.2.1. *Functional Unit and System Boundaries*

The definition of the functional unit has important implications for developing an LCA. The production of 1 kg of steel from primary materials, considering alloy composition, was taken as a functional unit in this study.

The life cycle stages considered in this study (Figure 3) corresponded to raw material acquisition, transports of these raw materials to the steel manufacturing plant and production processes for steel, as shown in Figure 1.

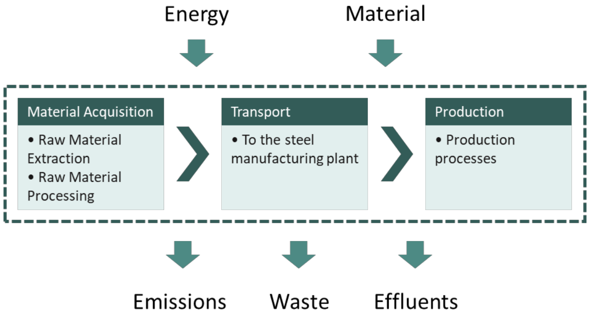


Figure 3. System boundaries

2.2.2. *Databases and Impact Categories*

The life cycle inventory was carried out through the EcoInvent v3.5 database, developed by the Swiss Centre for the Life Cycle Inventories. This database stands out as one of the most complete and highest quality at the European level.

The LCA was calculated according to two different methodologies of environmental impact calculation:

- ReCiPe 2016 EndPoint (H) V1.03 / World (2010) H/A
- CML-IA baseline V3.05 / EU25

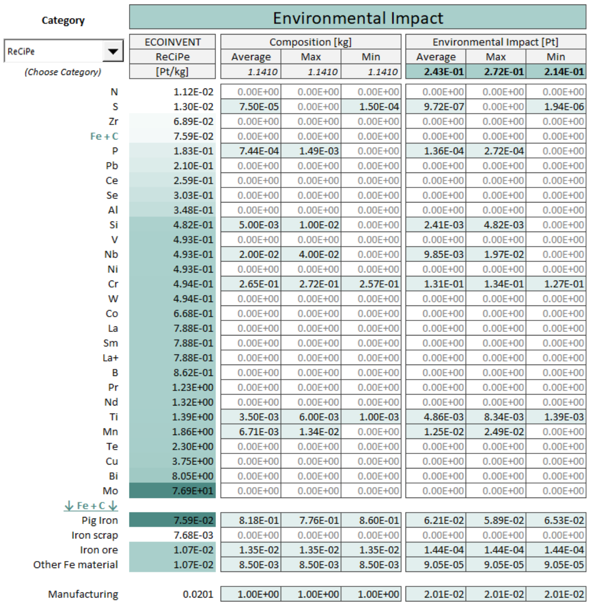
Both methodologies assess the environmental damage in different impact categories related to human health, available resources and ecosystems. However, each methodology has certain peculiarities.

ReCiPe 2016 methodology assess 18 impact categories and then weights them to a single value measured in points. The unique environmental impact value considerably simplifies the result interpretation (Huijbregts et al., 2017).

CML methodology offers the results in a disaggregated form, being able to assess more objectively the environmental impacts in each of the 11 impact categories included: Abiotic depletion, Abiotic depletion (fossil fuels), Global warming (GWP 100y), Ozone layer depletion (ODP), Human toxicity, Fresh water aquatic ecotoxicity, Marine aquatic ecotoxicity, Terrestrial ecotoxicity, Photochemical oxidation, Acidification and Eutrophication. This presentation of the results requires a more careful analysis of the results (Leiden University, 2016).

2.2.3. *Calculation methodology*

The calculation methodology can be considered a black box for the application user. Nevertheless, it is possible to view the Life Cycle Inventory modelling and Environmental Impact simulation for each of the 12 impact categories implemented, as shown in Figure 4.



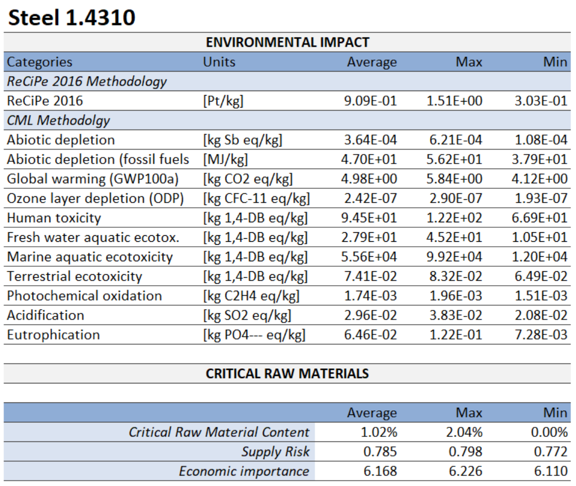
Category	Environmental Impact						
	ECOINVENT	Composition [kg]			Environmental Impact [Pt]		
ReCiPe	ReCiPe	Average	Max	Min	Average	Max	Min
(Choose Category)	[Pt/kg]	1.1410	1.1410	1.1410	2.43E-01	2.72E-01	2.14E-01
N	1.12E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
S	1.30E-02	7.50E-05	0.00E+00	1.50E-04	9.72E-07	0.00E+00	1.94E-06
Zr	6.89E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Fe + C	7.59E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
P	1.83E-01	7.44E-04	1.49E-03	0.00E+00	1.36E-04	2.72E-04	0.00E+00
Pb	2.10E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ce	2.59E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Se	3.03E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Al	3.48E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Si	4.82E-01	5.00E-03	1.00E-02	0.00E+00	2.41E-03	4.82E-03	0.00E+00
V	4.93E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nb	4.93E-01	2.00E-02	4.00E-02	0.00E+00	9.85E-03	1.97E-02	0.00E+00
Ni	4.93E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cr	4.94E-01	2.65E-01	2.72E-01	2.57E-01	1.31E-01	1.34E-01	1.27E-01
W	4.94E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Co	6.68E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
La	7.88E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sm	7.88E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
La+	7.88E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
B	8.62E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pr	1.23E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nd	1.32E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ti	1.39E+00	3.50E-03	6.00E-03	1.00E-03	4.86E-03	8.34E-03	1.39E-03
Mn	1.86E+00	6.71E-03	1.34E-02	0.00E+00	1.25E-02	2.49E-02	0.00E+00
Te	2.30E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cu	3.75E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Bi	8.05E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mo	7.69E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
↓ Fe + C ↓							
Pig Iron	7.59E-02	8.18E-01	7.76E-01	8.60E-01	6.21E-02	5.89E-02	6.53E-02
Iron scrap	7.68E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Iron ore	1.07E-02	1.35E-02	1.35E-02	1.35E-02	1.44E-04	1.44E-04	1.44E-04
Other Fe material	1.07E-02	8.50E-03	8.50E-03	8.50E-03	9.05E-05	9.05E-05	9.05E-05
Manufacturing	0.0201	1.00E+00	1.00E+00	1.00E+00	2.01E-02	2.01E-02	2.01E-02

Figure 4. Life Cycle Inventory modelling for ReCiPe 2016 methodology

2.3. Output data

As a result of the Life Cycle Inventory modelling, it is possible to simulate the Environmental Impact of steel production. By establishing three different models, three environmental impact results are obtained for each methodology or impact category. In the same way, the established models give a maximum and minimum content of critical raw materials, depending on the composition ranges.

These results can be represented in the data visualization sheet, shown in Figure 5.



Steel 1.4310

ENVIRONMENTAL IMPACT

Categories	Units	Average	Max	Min
ReCiPe 2016 Methodology				
ReCiPe 2016	[Pt/kg]	9.09E-01	1.51E+00	3.03E-01
CML Methodolgy				
Abiotic depletion	[kg Sb eq/kg]	3.64E-04	6.21E-04	1.08E-04
Abiotic depletion (fossil fuels	[MJ/kg]	4.70E+01	5.62E+01	3.79E+01
Global warming (GWP100a)	[kg CO2 eq/kg]	4.98E+00	5.84E+00	4.12E+00
Ozone layer depletion (ODP)	[kg CFC-11 eq/kg]	2.42E-07	2.90E-07	1.93E-07
Human toxicity	[kg 1,4-DB eq/kg]	9.45E+01	1.22E+02	6.69E+01
Fresh water aquatic ecotox.	[kg 1,4-DB eq/kg]	2.79E+01	4.52E+01	1.05E+01
Marine aquatic ecotoxicity	[kg 1,4-DB eq/kg]	5.56E+04	9.92E+04	1.20E+04
Terrestrial ecotoxicity	[kg 1,4-DB eq/kg]	7.41E-02	8.32E-02	6.49E-02
Photochemical oxidation	[kg C2H4 eq/kg]	1.74E-03	1.96E-03	1.51E-03
Acidification	[kg SO2 eq/kg]	2.96E-02	3.83E-02	2.08E-02
Eutrophication	[kg PO4--- eq/kg]	6.46E-02	1.22E-01	7.28E-03

CRITICAL RAW MATERIALS

	Average	Max	Min
Critical Raw Material Content	1.02%	2.04%	0.00%
Supply Risk	0.785	0.798	0.772
Economic importance	6.168	6.226	6.110

Figure 5. Results displaying

3. Case of study

In order to provide a clearer explanation of how the simulation tool works, as well as its applicability, the following case study is shown. The simulation of the environmental impact of three different steels used as raw material for the manufacture of steel elements in led luminaries has been carried out.

The three steels included in this case study are 1.4310, 1.0917 and 1.0347. They correspond to the categories of stainless steel, low-alloyed steel and unalloyed steel respectively. These would be the datasets chosen, in the case of using the Life Cycle Inventory models provided by EcoInvent. However, the simulation tool presented in this communication makes it possible to obtain a more accurate environmental impact, establishing a Life Cycle Inventory model based on the exact composition of each steel alloy. For this, it was only necessary to input the composition data obtained from standards, which are shown in Table 1.

Table 1. Composition ranges of steels.

Alloying element	1.4310 (1) Stainless	1.0917 (2) Low-alloyed	1.0347 (3) Unalloyed
Cr	16.0-19.0	-	-
Mn	2.0	1.2	0.45
Mo	0.8	-	-
N	0.1	-	-
Nb	-	-	-
Ni	6.0-9.5	-	-
P	0.045	0.12	0.035
S	0.015	0.045	0.035
Si	2.0	0.5	-
Ti	-	0.3	-
V	-	-	-
W	-	-	-

Standards: (1) EN10088-1:2015, (2) EN 10346:2015 y (3) EN 10152:2017

In this way, it is possible to simulate the environmental impact of the three steels by means of the simulation tool. The results obtained are shown in Table 2.

Table 2. Average Environmental impact under simulation tool model.

Impact category	Unit	1.4310 Stainless	1.0917 Low-alloyed	1.0347 Unalloyed
ReCiPe Methodology				
ReCiPe 2016	Pt	$9.09\boxed{\times 10^{-1}}$	$1.09\boxed{\times 10^{-1}}$	$9.60\boxed{\times 10^{-2}}$
CML Methodology				
Abiotic depletion	kg Sb eq.	$3.64\boxed{\times 10^{-4}}$	$1.61\boxed{\times 10^{-5}}$	$1.50\boxed{\times 10^{-6}}$
Abiotic depletion (fossil fuels)	MJ	$4.70\boxed{\times 10^{1}}$	$1.50\boxed{\times 10^{1}}$	$1.42\boxed{\times 10^{1}}$
Global warming (GWP100y)	kg CO_2 eq.	$4.98\boxed{\times 10^{0}}$	$2.09\boxed{\times 10^{0}}$	$2.01\boxed{\times 10^{0}}$
Ozone layer depletion (ODP)	kg CFC-11 eq.	$2.42\boxed{\times 10^{-7}}$	$8.86\boxed{\times 10^{-7}}$	$8.24\boxed{\times 10^{-8}}$
Human toxicity	kg 1,4-DB eq.	$9.45\boxed{\times 10^{1}}$	$8.30\boxed{\times 10^{1}}$	$7.69\boxed{\times 10^{-1}}$
Fresh water aquatic ecotox.	kg 1,4-DB eq.	$2.79\boxed{\times 10^{1}}$	$5.21\boxed{\times 10^{0}}$	$4.13\boxed{\times 10^{-1}}$
Marine aquatic ecotoxicity	kg 1,4-DB eq.	$5.56\boxed{\times 10^{4}}$	$1.50\boxed{\times 10^{3}}$	$1.27\boxed{\times 10^{3}}$
Terrestrial ecotoxicity	kg 1,4-DB eq.	$7.41\boxed{\times 10^{-2}}$	$3.06\boxed{\times 10^{-2}}$	$2.95\boxed{\times 10^{-3}}$
Photochemical oxidation	kg C2H4 eq.	$1.74\boxed{\times 10^{-3}}$	$1.20\boxed{\times 10^{-3}}$	$1.16\boxed{\times 10^{-3}}$
Acidification	kg SO2 eq.	$2.96\boxed{\times 10^{-2}}$	$7.02\boxed{\times 10^{-3}}$	$6.61\boxed{\times 10^{-3}}$
Eutrophication	kg PO4--- eq.	$6.46\boxed{\times 10^{-3}}$	$3.23\boxed{\times 10^{-3}}$	$3.04\boxed{\times 10^{-3}}$

As has been said before, the composition of steel has a significant influence on the result of environmental impact. For this reason, using this simulation tool based on steel composition, allows obtaining a more accurate impact results and being able to discretize between different steels of the same category (stainless, low-alloyed or unalloyed steel). To illustrate this, the following figures represent the variation of the environmental impact obtained by the simulation tool and those obtained with EcoInvent model.

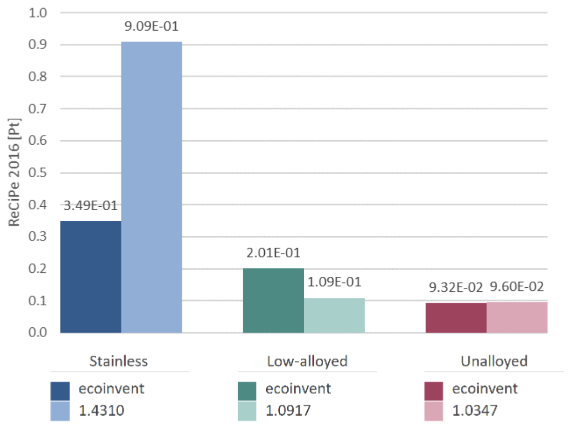


Figure 6. Environmental impact according to ReCiPe 2016 methodology.

It can be seen that in the case of ReCiPe 2016 methodology (Figure 6), the greatest difference is obtained in the case of stainless steel (+160.3%), due to the high amount of alloying elements that it includes, and especially because it includes Molybdenum, an alloying element with a high environmental impact. In the case of low-alloyed steel, making an accurate calculation based on the composition results in a lower impact than that obtained by EcoInvent, with a variation of -45.9%. In the case of unalloyed steel, the impact obtained is slightly higher (+3.0%).

The simulation tool allows quantify the presence of critical raw materials in steels. The results obtained from the case study are shown in Figure 7. Stainless steel is the steel with the highest content of CRM, although it only represents 1.02% of the total weight.

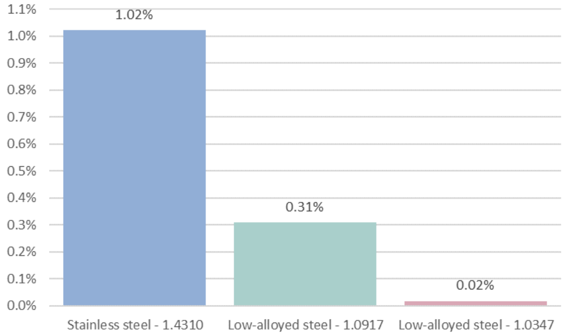


Figure 7. Critical Raw Material content.

4. Conclusions

The tool shown in this paper simulates the environmental impact of steel, by means of a LCA model based on the composition. It also performs a quantification of the content of critical raw materials. The results provided by this simulation tool allows designers to obtain a more accurate environmental impact calculation, and thereby make a more informed choice in relation to the material selection.

The easy use tool only requires entering the composition data of the steel to be analysed. The software is programmed to perform an LCA model and simulate the calculation of the environmental impact according to ReCiPe 2016 and CML methodologies.

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