

Supplementary Materials

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S1. Introduction

S1.1 LCA in the steelmaking sector

Steel production is characterized by the use of different materials, both raw and recycled, and it can be divided into two major production routes, depending on the type of process that is undertaken i.e. the primary route through Blast Furnace - Basic Oxygen Furnace and the secondary one through Electric Arc Furnace (EAF) [1]. Indeed, steel also constitutes one of the most efficiently recycled materials, which is therefore considered with interest in the field of Circular Economy [2]. Similar considerations arise from the possibility of recycling steel slag [3]. Some studies estimate that between 2050 and 2060, secondary steel production may surpass primary production [4], while others pointed out how the availability of steel scraps for secondary production will be strongly limited and incapable to substitute primary steelmaking entirely [5, 6]. In any case, the steel sector constitutes one of the largest energy consuming industry, associated with 6.7% of global anthropogenic CO₂ emissions which are expected to decrease, following the more and more restrictive regulations which are being set in place today [7]. However, relevant burdens are associated to other impact categories as well, such as water footprints [8]. Opportunities to reduce the steel sector environmental burdens have been analyzed, with some studies envisioning the creation of markets for green steel, the diffusion of emerging low carbon technologies, the closing of the steel cycle loops and the incorporation of material efficiency measures into the decarbonization portfolio [9, 1].

When carrying out an LCA within this field, methodological issues arise in how to account for the recyclability of such materials, and which impacts should be assigned to recycled steel scraps. Different models were proposed, based on the distinction between attributional and consequential LCA models and the consideration of one or multiple life cycles within the LCA calculations [10, 11, 12]. The choice of selected method for allocation of recycling leads to wide discrepancies in LCA results: for instance, the global warming impact of hot-rolled strip, with a recycling rate of 95%, was estimated to vary between 2 and -2 kg CO₂-eq per kg of steel [12]. Here, the flexibility provided by an LCA tool can help dealing with multiple approaches for modelling recycling.

This sector is also interesting in the LCA field due to the general lack of data regarding steel production processes [7]. Steel production plants employ different raw materials such as iron ores, scraps and ferroalloys. Concerning the latter, currently a few studies identified LCA impacts associated to the most widely used alloys: Ferromolybdenum (FeMo) [13], ferromanganese (FeMn) [14, 15], ferronickel (FeNi) [16, 15], ferrosilicon

(FeSi) [15]. The ecoinvent database (version 3.6) [17] provides data for FeMn, FeNi, FeSi, ferrochromium (FeCr) as well. However, many more types of iron alloys may be used in the steelmaking sector, such as ferrotitanium (FeTi), ferrotungsten and ferrovanadium [15].

S2. Methods

S2.1 Processing in the Spreadsheet module

S2.1.1 Harmonization of time resolution across all foreground LCI data

Stack emissions and scraps consumption are not monitored at the monthly level, even if the company has this objective in the near term.

Concerning stack emissions: apart from particulates, pollutants concentrations (NO_x, SO_x, CO and NMVOC) are currently monitored twice a year, according to the Italian legal requirements. However, particulates concentrations, together with flue gases and flow rates are monitored with a continuous measurement system (SME), which provides data at much smaller time intervals. Such information can be used, together with the monthly working hours of the plant, to compute the total amount of pollutants emitted in air within the selected timestep, according to equation 1:

$$Emission_{i,t}[g] = Concentration_{i,t*}[g/Nm^3] * FlowRate_{i,t}[Nm^3/h] * WorkingHours_t[h] \quad (1)$$

with the timesteps $t* \neq t$, being them related to a different time resolution ($t*$ is semestral, t is monthly) and i representing the emitted compound; g =grams, Nm^3 =normal cubic meter, h =hours. Such equation assumes the concentration of pollutants to remain equal over the selected timesteps. In order to provide more stable data, such concentration may also be averaged across different measurements data: e.g. using the rolling average of the last 4 measurements.

Concerning steel scraps: consumption data are only collected at the yearly level. In this case, consumption data were allocated across the months based on the amount of steel billets produced, as the following equation shows:

$$Scraps_t = Scraps_{t*} * Production_t / \sum_{t=1}^{12} (Production_t) \quad (2)$$

with the timesteps $t* \neq t$, being them related to a different time resolution ($t*$ is yearly, t is monthly).

S2.1.2 Change in units of measure

The consumption of oxygen was provided in normal cubic meters (0°C and 1 atmosphere), while the consumption of nitrogen and argon was provided in technical cubic

meters (15°C and 98067 Pa). However, the reference flow of the related ecoinvent datasets is expressed in kg. Therefore, according to the ideal gases law, the conversion factors between these units were computed.

S2.1.3 Calculation of dependent items

Specific types of data can be dependent on other data. CO₂ emissions are dependent on the amount of natural gas burnt each month; thus, once the ratio of kg CO₂/m³ natural gas is known, the rows related to CO₂ emissions can be easily added to the *Consumption/emission* sheet of the Spreadsheet module, with the same level of detail as natural gas. The same applies to transport services, which are dependent on the amount of materials consumed. Once the distances are known, the rows related to transport services can be easily added to the *Consumption/emission* sheet of the Spreadsheet module, with the same level of detail as the consumed materials.

S2.1.4 Calculation of specific items

The total quantity of iron alloys was available at the monthly level, the consumption of each specific iron alloy was not available from the primary data of this study. Therefore, the shares of every single alloy were kept equal to the yearly value, to compute monthly consumptions for every iron alloy (IA), as shown by the following equation

$$IA_{f,t} = \sum_{f=1}^F (IA_{f,t}) * IA_{f,t*} / \sum_{f=1}^F (IA_{f,t*}) \quad (3)$$

with f being a specific iron alloy, F being the number of different iron alloys consumed and with the timesteps $t* \neq t$, being them related to a different time resolution (t^* is yearly, t is monthly).

S2.2 Processing in the Coding module

S2.2.1 Inclusion of co-products produced by the factory

According to the EPD rules, this step must be dealt with by means of an allocation of the LCI to the different products of the company. Indeed, in addition to the main steel products, some co-products are sold to the external market, too. In particular for our case, the latter are related to some types of wastes sent to recycling and to the excess heat, which is provided to the municipality via district heating during winter months. In accordance to the International EPD system rules and due to the different physical units of the co-products (respectively mass and energy), an economic allocation was performed, computing the revenues associated to the main products and co-products.

Therefore, the LCI is allocated to the main steel products with the following equation:

$$LCI_{i,j,t} = PreliminaryLCI_{i,j,t} * Revenues_{steel,t} / (Revenues_{steel,t} + \sum_{k=1}^K (Revenues_{co-products,t})) \quad (4)$$

with k being the considered co-product and K the total number of products, i the Flow key index, j the considered main steel product (one of the nine products outlined by figure 1, t the considered timestep. Currently, the main steel products dominate the revenues, yet the company aims at further increasing the share of valuable wastes sold externally over the years. If wastes are sold as co-products, then the related revenues will increase and so will the fraction of total impacts allocated to co-products, decreasing the impacts associated to steel products. This makes the use of equation 4 further useful. In other organizations, co-products may also be related to excess electricity exported to the national grid.

The way equation 4 is structured depends on label-specific rules. For instance, depending on the rules defined by the selected environmental label, the inclusion of co-products may follow other approaches with respect to equation 4, such as system expansion and crediting, which belong the ISO 14044 hierarchy [18].

S2.2.2 Treatment of consumptions which are common across products

This is the case for auxiliary services for heating and lighting or some types of waste streams (e.g. total waste plastics produced by the offices), which are defined at plant level, thus they are in common across all products. According to the EPD rules, this step must be dealt with the definition of allocation parameters, which affect how common consumptions are divided between different products. These data must be allocated to all the different main products of the company. Within our case study, we allocated plant-level consumptions to the different production unit based on the mass of the selected products, according to the following equation:

$$AuxiliaryLCI_{i,j,t} = AuxiliaryLCI_{i,t} * (Product_{j,t} / \sum_{j=1}^N (Product_{j,t})) \quad (5)$$

with N being the number of all products. The *Auxiliary* terms will then be summed up with the *LCI* terms of equation 4, to obtain the total LCI for each product. The same equation could be used for other types of allocations: in case of an economic allocation, the *Production* terms would be related to the revenues, instead of the mass of the selected product.

S2.2.3 Specific calculations

A percentage of the total steel billets entering the rolling mill process is discarded. Therefore, more than 1 ton of steel billets is needed to produce 1 ton of hot-rolled steel. This inefficiency percentage varies over time and it is accounted for with a factor

higher than 1, which is applied to the steelmaking production unit, for hot-rolled and thermally treated products.

S3. Results

The following section provides additional information on the analyses shown in the main paper. It is articulated into three parts, in accordance to the three RQ of the main paper.

S3.1. RQ1: Dynamic LCA results

The following table describes the impact categories and related acronyms and units which are used in this section. This section digs into a simplified statistical analysis of the variability of monthly LCA results, across products, impact categories and main contributors. The processes are grouped according to the classification of table 3 of the main paper.

Impact category	Impact category (abbreviation)	Unit
Abiotic depletion potential – Elements	ADP, elements	kg Sb-eq
Abiotic depletion potential – Fossil fuels	ADP, fossil fuels	MJ
Acidification potential	AP	kg SO ₂ -eq
Eutrophication potential	EP	kg PO ₄ ³⁻ -eq
Global warming potential	GWP	kg CO ₂ -eq
Photochemical oxidant formation potential	POFP	kg NMVOC-eq
Primary energy resources – Non-renewable	Non-Ren LHV CED	MJ
Primary energy resources – Renewable	Ren LHV CED	MJ
Water scarcity potential	WSP	m ³ -eq

Table S1: Description of impact categories selected for the visualization of results. The categories are taken from the International EPD system scheme.

The first analysis aims at understanding which drivers contribute more to the variability of total LCA results. The following two figures aim at correlating the variability of single drivers (on the y-axis) with the variability of total LCA results (on the x-axis). On the y-axis, results are relative to the yearly value of the selected process group. This means that, for instance, the first top chart on the left shows the monthly results of the Energy group, relative to the yearly LCA results of the Energy group, in the ADP, elements category. On the x-axis, the monthly total LCA results (i.e. the sum of all contributions) are shown, relative to the yearly value of total LCA results. In this way, it can be outlined which drivers contribute more to the variability of total LCA results:

the more the displayed scatterplots align on a straight line, the more relevant is the variability of the selected driver.

In the ADP, elements category, most of the variance of total LCA results is explained by the variability of the Materials group and the same happens in most of the impact categories. In the WSP category, most of the variance of total LCA results is explained by the variability of the Consumables group, in which water withdrawals are included. In the ADP, fossil fuels, Non-Ren CED and GWP categories, a remarkable portion of the variance of total LCA results is explained by the variability of the Energy group, due to the relevance of electricity supply in these categories. The remaining drivers show a negligible influence on the variability of total LCA results. Then, it must be remarked that the Materials and Upstream transport groups are partially dependent, since transport depend on the amount of consumed materials. The Emissions driver is only defined in 4 impact categories due to the fact that elementary flows comprised in this group do not contribute to the other categories.

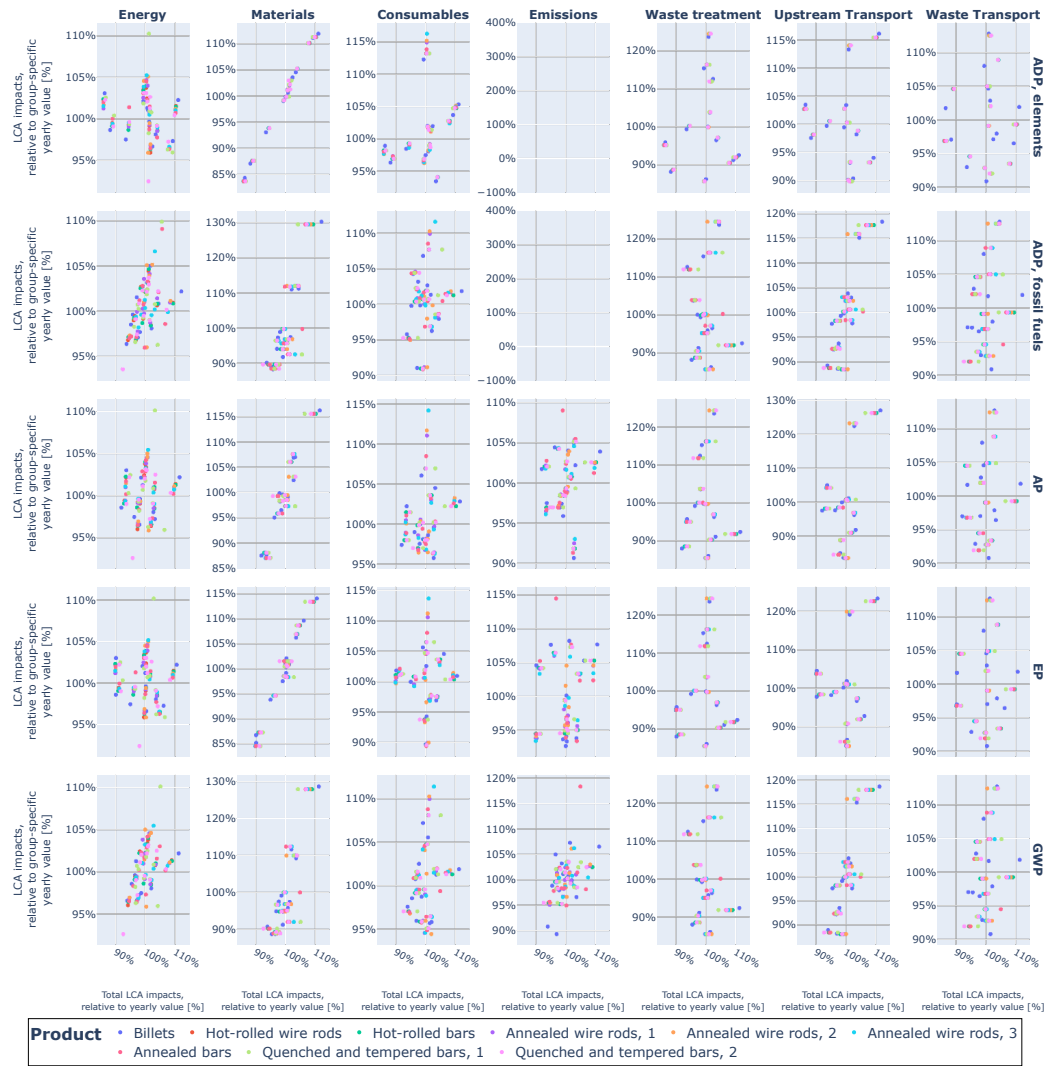


Figure S1: Scatterplots of monthly LCA results of different drivers, for all the products and 5 impact categories. On the x-axis, the total LCA impacts, relative to the yearly value. On the y-axis, results are relative to the yearly value of the selected process group, for the related product and impact category.

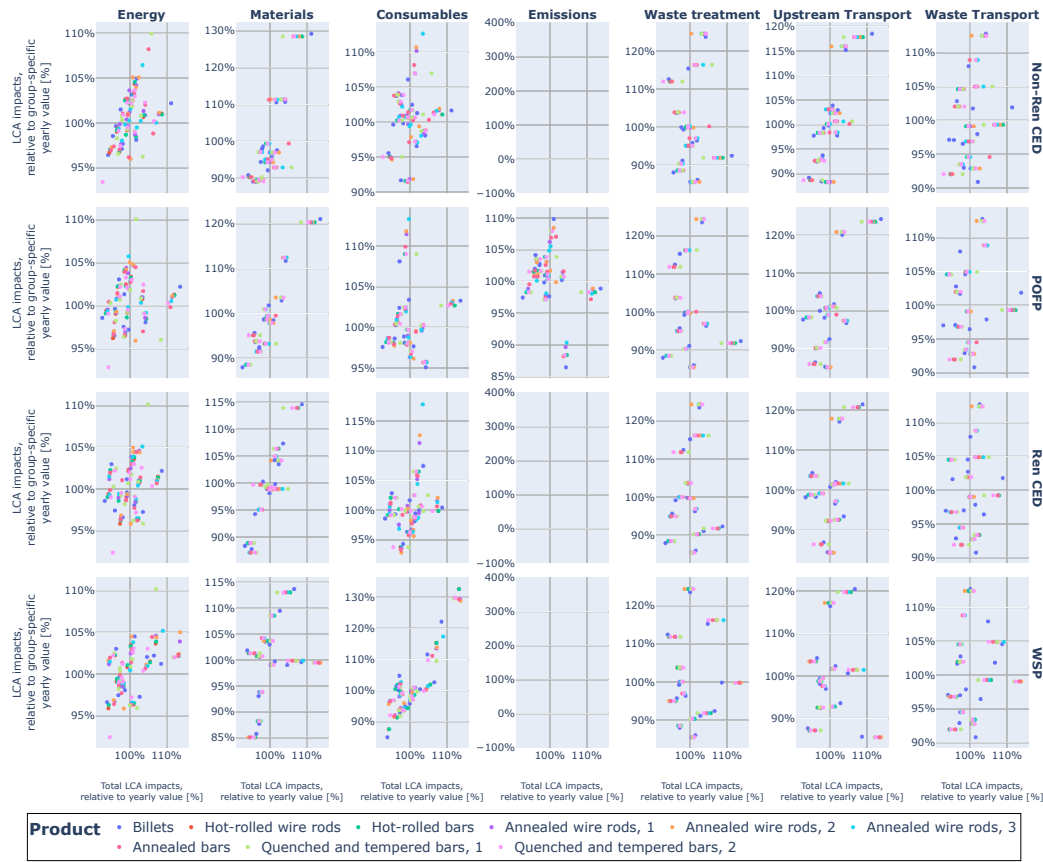


Figure S2: Scatterplots of total monthly LCA results, for all the products and 4 impact categories. Results are relative to the yearly value of the selected process group, for the related product and impact category.

The following 5 charts then compute the R^2 measure of the different process groups, with respect to total LCA results. R^2 represents the portion of the variance of the dependent variable (i.e. total LCA results) that is explained by independent variables (single process groups). It can be clearly seen that the Materials group shows the highest R^2 across impact categories, apart from WSP, followed by the Upstream transport group, which is partially dependent on the Materials group itself. The Energy group also shows a relevant R^2 in some impact categories (GWP; Non-Ren CED; ADP, fossil fuels) and the Consumables group show the highest R^2 for the WSP category.



Figure S3: R^2 measures for the variance of total LCA results explained by different groups of processes (Medium detail), for three different products, across the selected categories outlined by table S1



Figure S4: R^2 measures for the variance of total LCA results explained by different groups of processes (Medium detail), for three different products, across the selected categories outlined by table S1



Figure S5: R^2 measures for the variance of total LCA results explained by different groups of processes (Medium detail), for three different products, across the selected categories outlined by table S1



Figure S6: R^2 measures for the variance of total LCA results explained by 3 different groups of processes (Medium detail), for all the products, across the selected categories outlined by table S1



Figure S7: R^2 measures for the variance of total LCA results explained by 4 different groups of processes (Medium detail), for all the products, across the selected categories outlined by table S1

The following figures display the standard deviation of single process groups. The standard deviation of the Materials group does not vary across products (apart from Annealed wire rods 2 and 3, since they were not produced in some months), since most of the materials are consumed in the steelmaking production unit and they are thus carried by all processes. The standard deviation of total results is very similar to the standard deviation of the Materials group. The Materials group shows the highest standard deviations, followed by the Energy and Consumables groups, apart from WSP category which is dominated by Consumables. The standard deviation of the Energy group increases towards quenched and tempered bars, due to the higher consumption of electricity.

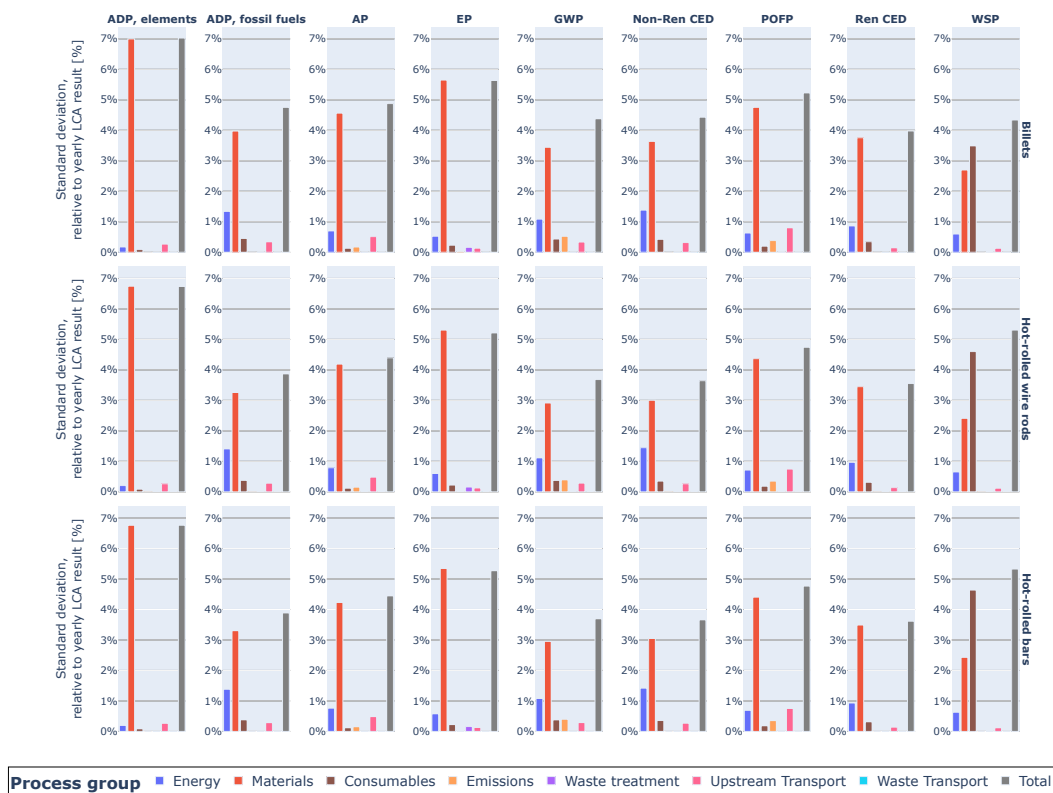


Figure S8: Standard deviation, relative to yearly LCA results, of all the different groups of processes (Medium detail) and of the total LCA results, for 3 products, across the selected categories outlined by table S1. Results are expressed per unit of steel; while the numerator of the unit of results depends on the selected impact category and it can be seen in the Unit column of table S1

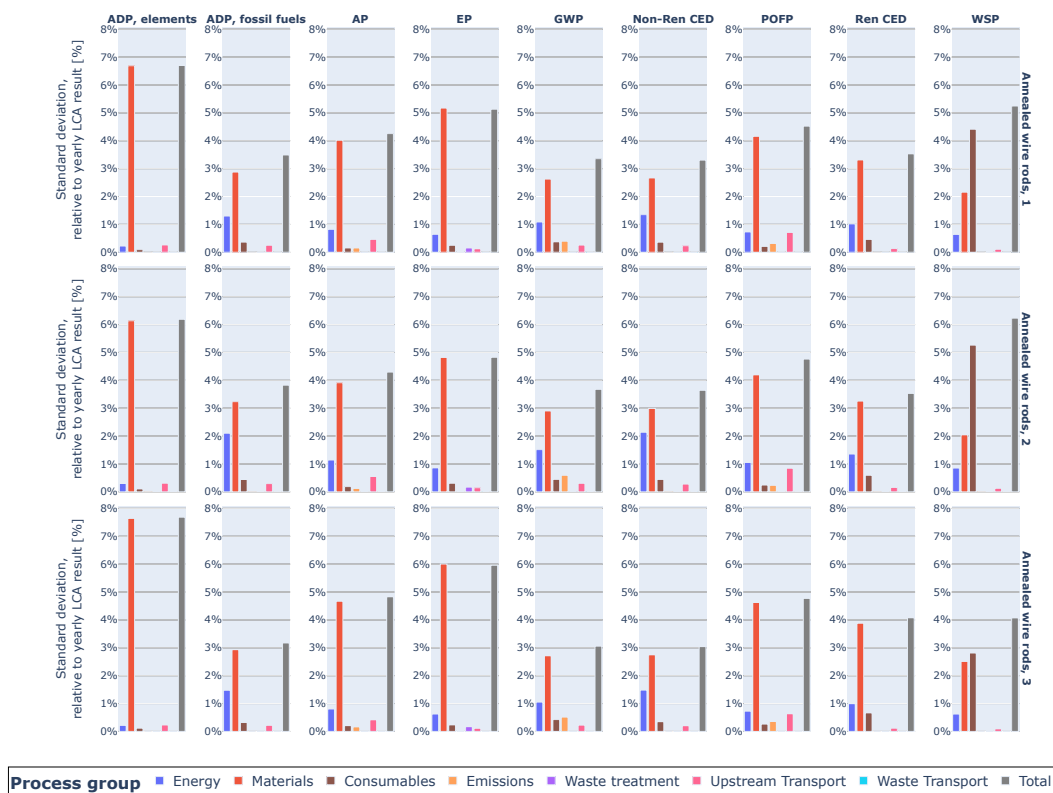


Figure S9: Standard deviation, relative to yearly LCA results, of all the different groups of processes (Medium detail) and of the total LCA results, for 3 products, across the selected categories outlined by table S1. Results are expressed per unit of steel; while the numerator of the unit of results depends on the selected impact category and it can be seen in the Unit column of table S1

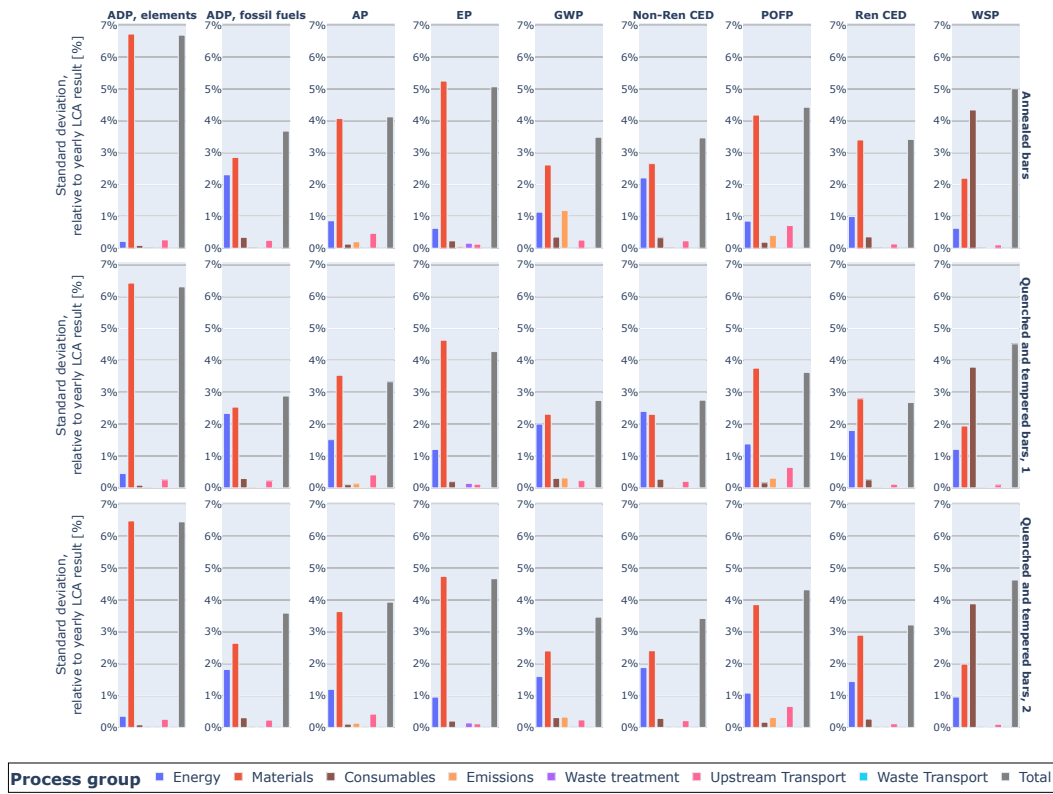


Figure S10: Standard deviation, relative to yearly LCA results, of all the different groups of processes (Medium detail) and of the total LCA results, for 3 products, across the selected categories outlined by table S1. Results are expressed per unit of steel; while the numerator of the unit of results depends on the selected impact category and it can be seen in the Unit column of table S1

The variability of LCA results that was found is comparable with results by Moon et al. [19] on steel slab, who found an average yearly result of 1303 kg CO₂-eq/ton, with monthly results that varied between 1276 kg CO₂-eq/ton to 1334 kg CO₂-eq/ton and 18 kg CO₂-eq/ton of standard deviation. In their study, the ratio of standard deviation by yearly average is 1.4%. In our case, the ratio of standard deviation by yearly average is between 2.7% and 4.4% across the analysed products, for the same impact category (see the Total group in figure S11 of the supplementary materials), while values are slightly higher for other impact categories (up to 7.7% in the Abiotic depletion, elements category).

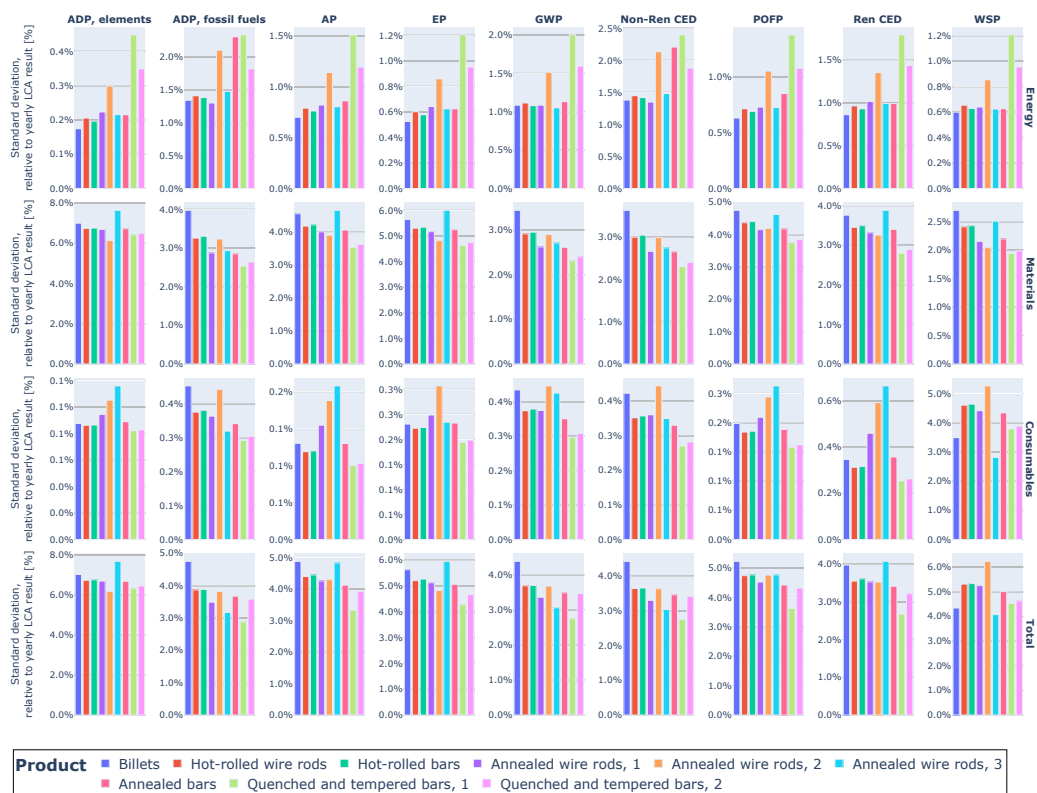


Figure S11: Standard deviation, relative to yearly LCA results, of 3 different groups of processes (Medium detail) and of the total LCA results, for all the products, across the selected categories outlined by table S1. Results are expressed per unit of steel; while the numerator of the unit of results depends on the selected impact category and it can be seen in the Unit column of table S1



Figure S12: Standard deviation, relative to yearly LCA results, of 4 different groups of processes (Medium detail), for all the products, across the selected categories outlined by table S1. Results are expressed per unit of steel; while the numerator of the unit of results depends on the selected impact category and it can be seen in the Unit column of table S1

The following figures outline the highest variations of monthly LCA results, for different process groups. Variations are relative to the yearly value of total LCA results (which are constituted by the sum of LCA results of 7 different groups), according to the following equation:

$$Yaxisvalue_{i,j,z} = (LCA_{i,j,z} - LCA_{i,j,z,yearly}) / \sum_{i=1}^7 (LCA_{i,j,z,yearly}) \quad (6)$$

with i being the selected process group, j the selected product and z being the selected impact category. $LCA_{i,j,z}$ is the highest or lowest monthly LCA result of a selected process group, for a selected product and impact category.

As can be seen, the Materials group shows the highest variations, followed again by the Energy and Consumables groups, apart from the WSP category which is dominated by Consumables. The relative variations of the Materials group slightly decrease when moving towards thermally treated products, since most of the materials are consumed in the steelmaking production unit. Therefore, the $LCA_{i,j,z}$ term for Materials does not increase from steel billets to thermally treated steel, while the $LCA_{i,j,z,yearly}$ instead does, due to the higher impacts of these products. The opposite happens for the Energy and Emissions groups, since thermally treated steel is associated to a higher

consumption of energy and emissions of greenhouse gases. As happened with the standard deviation, the highest variations of the Materials group are similar to the highest variations of the total LCA results.



Figure S13: Highest variations of monthly LCA results, with respect to the yearly value of the selected process group, for different groups of processes (Medium detail) and for the total LCA results, for three different products, across the selected categories outlined by table S1. The variations are relative to the yearly value of total LCA results of the related product and impact category.



Figure S14: Highest variations of monthly LCA results, with respect to the yearly value of the selected process group, for different groups of processes (Medium detail) and for the total LCA results, for three different products, across the selected categories outlined by table S1. The variations are relative to the yearly value of total LCA results of the related product and impact category.

In the GWP chart of the quenched and tempered bars,1 product, the highest variations of the Energy and Materials groups are similar.



Figure S15: Highest variations of monthly LCA results, with respect to the yearly value of the selected process group, for different groups of processes (Medium detail) and for the total LCA results, for three different products, across the selected categories outlined by table S1. The variations are relative to the yearly value of total LCA results of the related product and impact category.

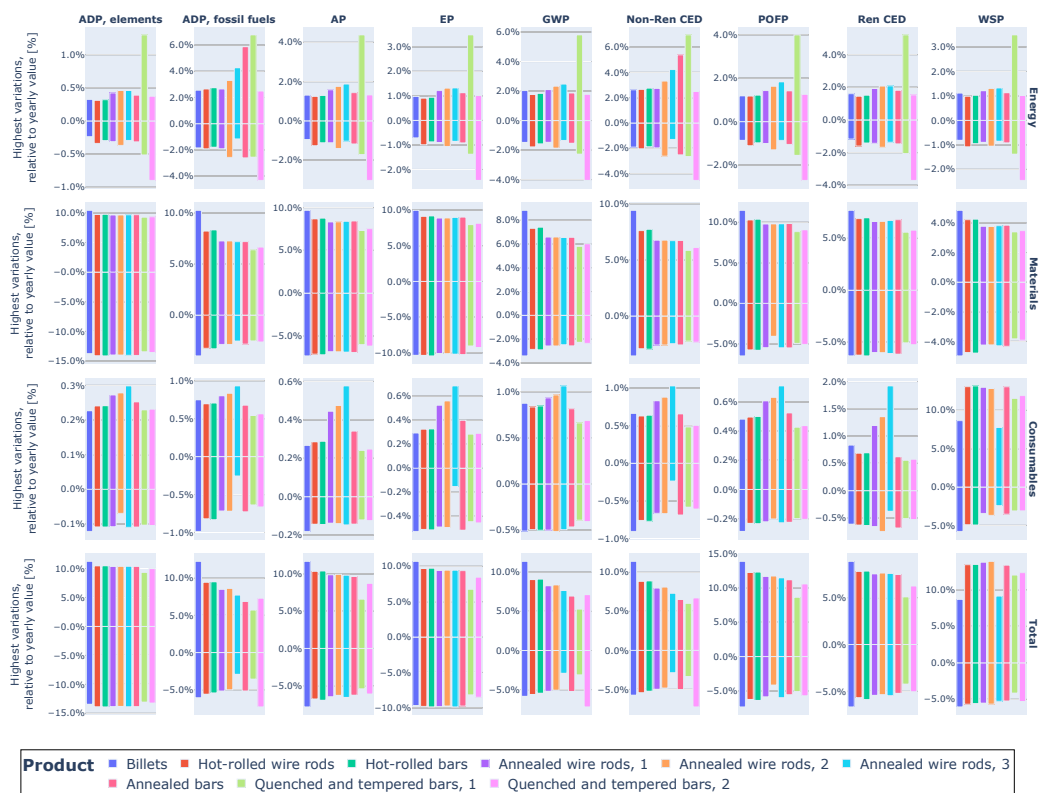


Figure S16: Highest variations of monthly LCA results, with respect to the yearly value of the selected process group, for 3 groups of processes (Medium detail) and for the total LCA results, for all different products, across the selected categories outlined by table S1. The variations are relative to the yearly value of total LCA results of the related product and impact category.

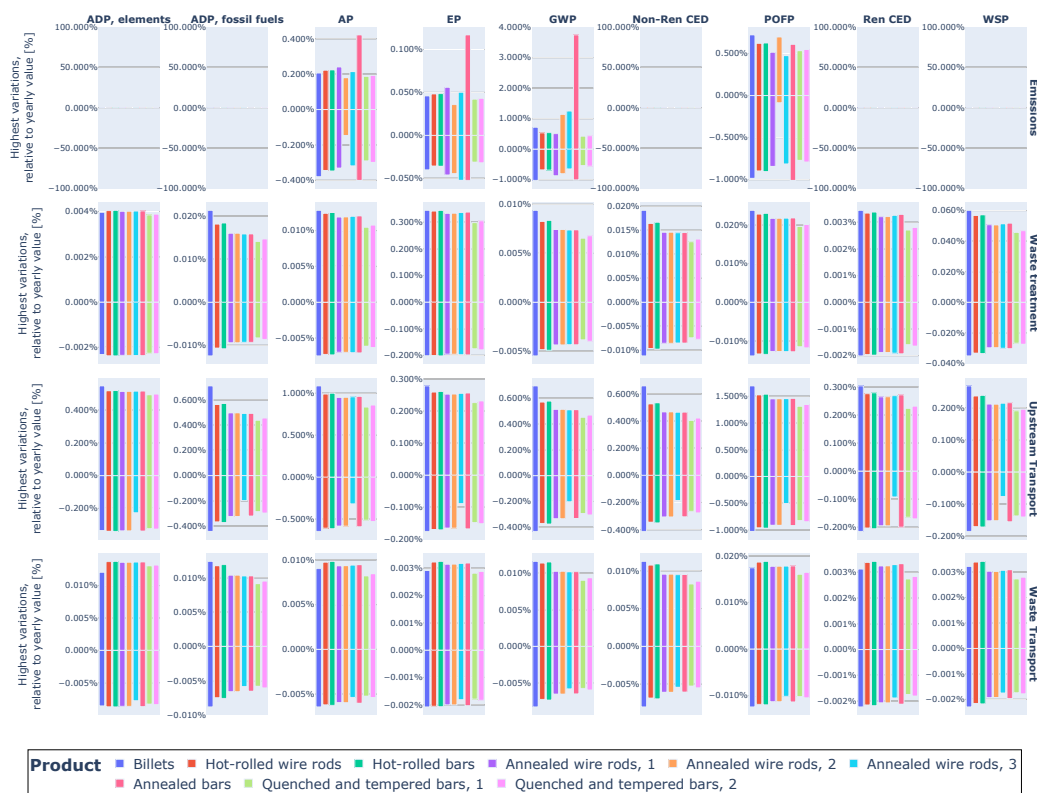


Figure S17: Highest variations of monthly LCA results, with respect to the yearly value of the selected process group, for 4 groups of processes (Medium detail), for all different products, across the selected categories outlined by table S1. The variations are relative to the yearly value of total LCA results of the related product and impact category.

S3.2. RQ2: Variability due to background datasets, LCIA methods and LSRs

The *molybdenite mine operation* process is multifunctional and produces both *molybdenite* and *copper concentrate, sulfide ore*. The ecoinvent database provides the prices associated to both products, which are respectively equal to 37.5 EUR2005 and 0.534 EUR2005 per kg of product. This means that the unitary impacts associated to *molybdenite* are $37.5/0.534=70$ times higher than the unitary impacts associated to *copper concentrate, sulfide ore*, which is the reason behind such a high impact for the production of FeMo alloy. If a mass-based allocation was instead chosen, the unitary impacts of both *molybdenite* and *copper concentrate, sulfide ore* products would be equal. Figure S18 then shows the related variations of total LCA results, for steel billets, due to the variations in unitary impacts of the selected secondary datasets.

Figures S19 and S20 show results for the water consumption categories respectively of the International EPD system scheme and ILCD methods (see the discussion on table 5 of the main paper). It can be seen that the two methods map completely different elementary flows.

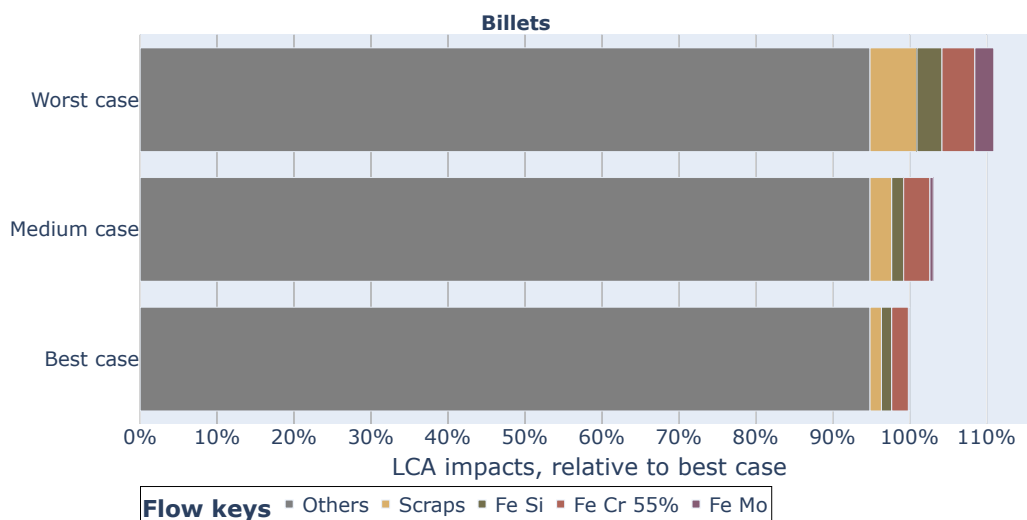


Figure S18: Comparison of yearly LCA results for steel billets, for the GWP category, across different cases of secondary datasets for modelling the background system, for steel scraps, FeMo, FeCr and FeSi, presented in table 4 of the main paper. These Flow keys are explicitly highlighted with different color bars, while the grey bar is related to the other processes which are left unchanged. Results are relative to the best case values.

Water scarcity		
F Water	Emission to water / ground water	-42.95000 m3 eq/m3
F Water	Emission to water / surface water	-42.95000 m3 eq/m3
F Water	Emission to water / unspecified	-42.95000 m3 eq/m3
F Water, cooling, unspecified natural origin	Resource / in water	42.95000 m3 eq/m3
F Water, lake	Resource / in water	42.95000 m3 eq/m3
F Water, river	Resource / in water	42.95000 m3 eq/m3
F Water, turbine use, unspecified natural origin	Resource / in water	42.95000 m3 eq/m3
F Water, unspecified natural origin	Resource / in water	42.95000 m3 eq/m3
F Water, unspecified natural origin	Resource / in ground	42.95000 m3 eq/m3
F Water, well, in ground	Resource / in water	42.95000 m3 eq/m3
F Water, well, IT	Resource / unspecified	44.88000 m3 eq/m3

Figure S19: Characterized elementary flows for the Water Scarcity category of the International EPD system scheme. Screenshot from OpenLCA software.

Impact factors: ILCD 2.0 2018 midpoint				
Impact factors				
Impact category resources - dissipated water				
Flow	Category	Flow property	Factor	Unit
Water	Emission to air/high population density	Volume	42.95	m3 water-Eq/m3
Water	Emission to air/low population density	Volume	42.95	m3 water-Eq/m3
Water	Emission to air/low population density, long-term	Volume	42.95	m3 water-Eq/m3
Water	Emission to air/lower stratosphere + upper tropos...	Volume	42.95	m3 water-Eq/m3
Water	Emission to air/unspecified	Volume	42.95	m3 water-Eq/m3

Figure S20: Characterized elementary flows for the ILCD 2.0 2018 midpoint method. Screenshot from OpenLCA software.

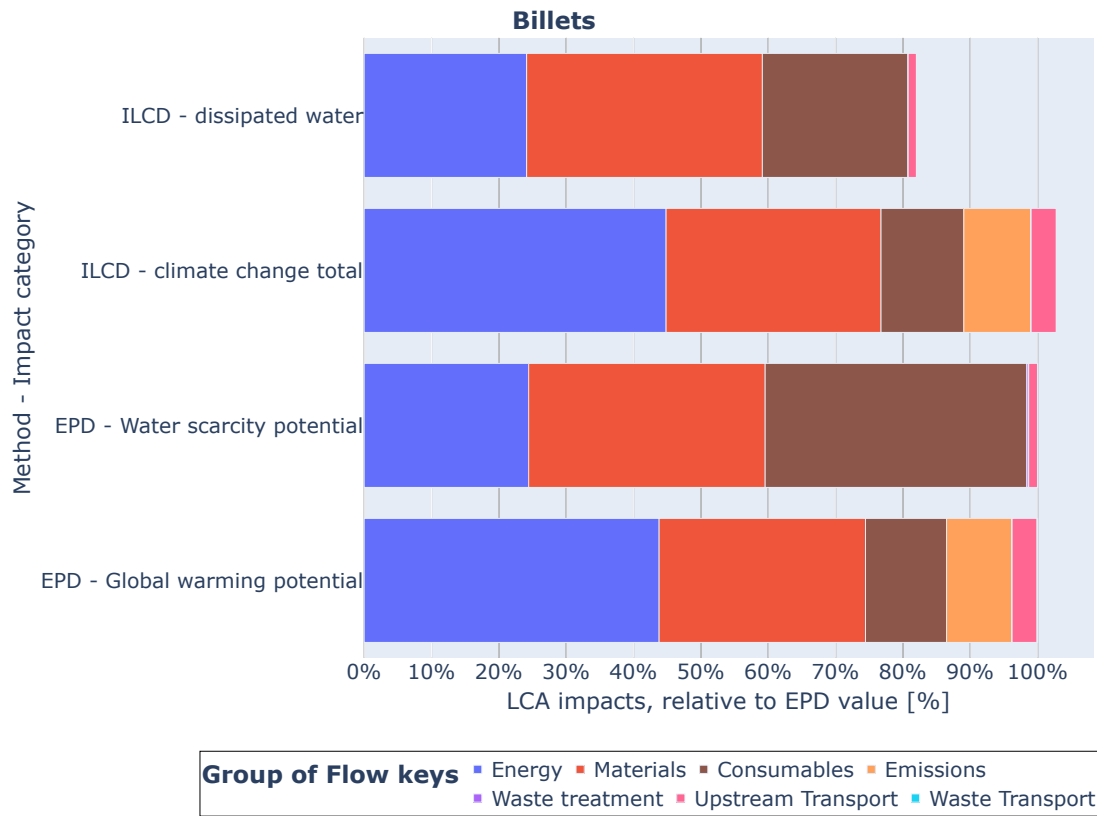


Figure S21: Comparison of yearly LCA results for steel billets, for the GWP category, across two categories related to water consumption and global warming, for the EPD and ILCD 2.0 midpoint LCIA methods. Flow keys are grouped according to the classification presented in table 3 of the main paper. Results are relative to the EPD value, which is thus set to 100%. The contributions of different groups of drivers are outlined with different colours.

S3.3. RQ3: Presentation of dashboards visualizations

Figure S22 presents an extract of the dashboard shown in figure 5 of the main paper, yet for the Water scarcity potential category. In this figure, LCA results for the left chart show different temporal dynamics with respect to the Global warming potential category, with the month of December showing the highest results. Moreover, the chart on the right outlines that the contribution of Consumables is higher, with respect to figure 5 of the main paper.

Then, figures S23 and S24 present an extract of the dashboard shown in figure 7 of the main paper, yet with other settings. In the first figure, the best month was selected, while in the second the worst month was selected. As can be seen, the best performing month changes across impact categories and products, while the worst month is always related to June. Results are displayed by product families, not by single products: for instance, if the only quenched and tempered bars, 1 are considered, the worst month is August and not June (see figure 3 of the main paper).

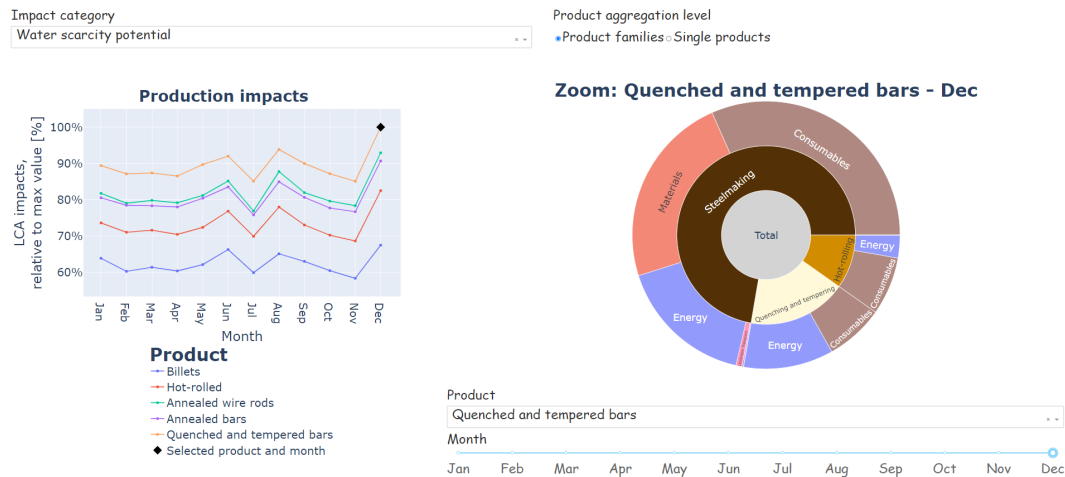


Figure S22: Screenshot extracted from a dashboard of the Visualization module, showing a line chart comparison of monthly LCA results for a selected impact category, for different products, on the left, presented in figure 5 of the main paper. With respect to the main paper, here the Water Scarcity Potential category was selected from the settings on the top-left part of the dashboard. The other characteristics remain the same as explained in the paper.

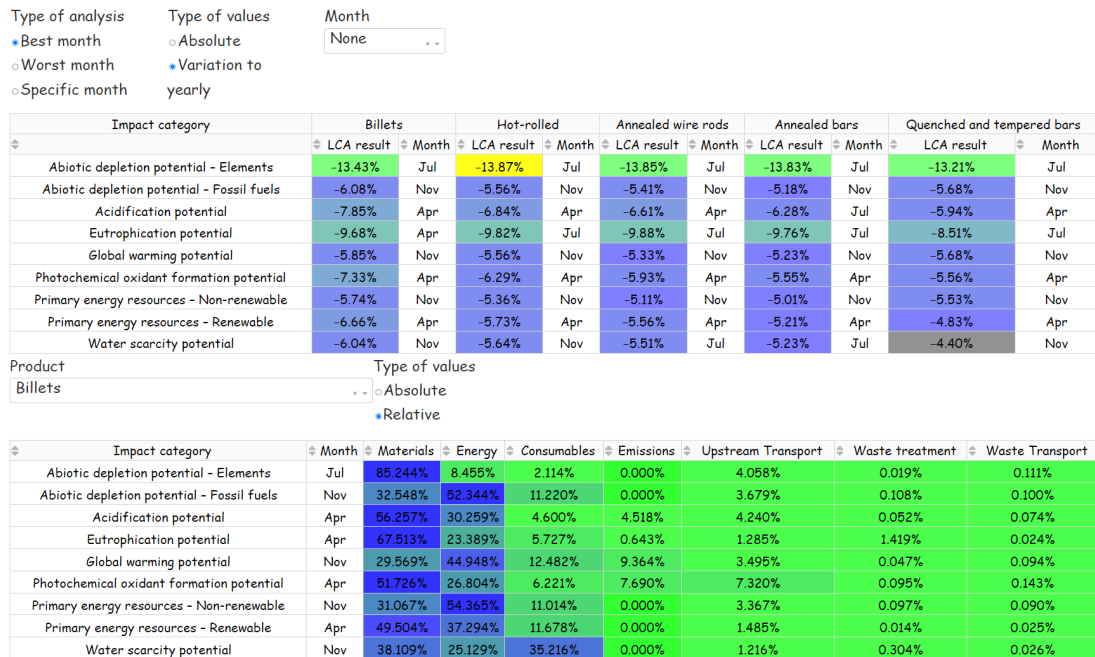


Figure S23: Screenshot from a dashboard for the comparison of LCA results across different impact categories (rows of the two tables), presented in figure 7 of the main paper. With respect to the main paper, here the best month was selected from the settings on the top-left part of the dashboard. The other characteristics remain the same as explained in the paper.

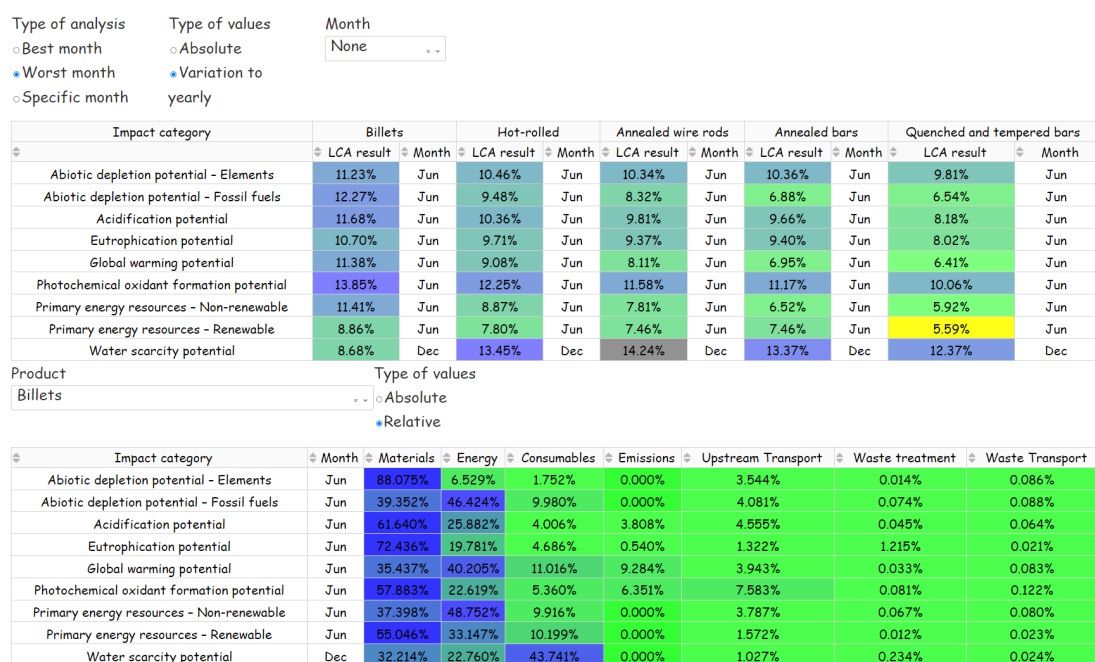


Figure S24: Screenshot from a dashboard for the comparison of LCA results across different impact categories (rows of the two tables), presented in figure 7 of the main paper. With respect to the main paper, here the worst month was selected from the settings on the top-left part of the dashboard. The other characteristics remain the same as explained in the paper.

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