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Integrating optimization and LCA models in the steelmaking process: insights from the ALCHIMIA project

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Abstract

Improving the sustainability of the steelmaking sector is a challenging task because steelmakers are expected to meet environmental targets and strict quality requirements that depend on the final application of the product. Recycling steel in electric arc furnaces (EAFs) is a well-established circular practice that helps reducing the environmental impact of steelmaking. However, an optimal combination of different scrap types and additions, along with minimum electricity and gas consumption during the melting phase, is necessary to ensure high quality and environmental performance of final products. The process input mix can be improved by exploiting optimization tools and Life Cycle Assessment (LCA) to minimize a multi-objective function including environmental impacts, constrained by technical requirements of steel and process operating conditions. The paper presents a methodology to transform "traditional" LCA into an "optimized LCA approach", focusing on how Life Cycle Inventories and Life Cycle Impact Assessment can be associated to optimization variables or inputs, depending on steelmakers' ability to affect EAF-based steelmaking operational parameters. The discussion highlights opportunities and limitations of integrating LCA and optimization methodologies within the framework of a real-world case study carried out in the European project ALCHIMIA.

Keywords: Life Cycle Assessment, Electric Arc Furnace, steel scrap, optimization

Nomenclature

AP	Acidification Potential
BF	Blast Furnace
BOF	Basic Oxygen Furnace
CED	Cumulative Energy Demand
DEA	Data Envelopment Analysis
EAF	Electric Arc Furnace
GWP	Global Warming Potential
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LF	Ladle Furnace
MILP	Mixed Integer Linear Programming

1. Introduction

Steelmaking is one of the most critical industrial sectors globally, as steel is extensively used in manufacturing processes. However, the steelmaking industry is known to have significant environmental burdens, prompting numerous research projects aimed at mitigating these impacts [1]. In this context, the Life Cycle Assessment (LCA) methodology has become increasingly important in scientific literature and international policies, as evidenced by the extensive number of studies on this topic [2]. In particular, LCA has been applied to quantify the potential environmental impacts of the production of primary steel in blast furnaces (BFs) and basic oxygen

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furnaces (BOFs), as well as to secondary steel production in Electric Arc Furnaces (EAFs) [2].

Research shows that while secondary steel recycling generally has a lower environmental impact than primary steel production [3], it still presents considerable environmental challenges [2]. For instance, the Global Warming Potential (GWP) of primary steel from BF-BOF ranges between 1.0 and 2.3 kg CO_2 eq per kg, whereas the greenhouse gas emissions associated with EAF range from 0.74 to 0.77 kg CO_2 eq per kg [2]. However, the comparison of the potential environmental impact between primary and secondary steel largely depends on the specific impact category being analyzed [2]. Moreover, existing LCA studies indicate that one of the primary contributors to the environmental impact of EAFs is electricity consumption, which is notably influenced by the composition of materials melted in the furnace [3]. These materials, mainly consisting of scrap and ferroalloys, are added to meet the quality standards required by customers [4]. Additionally, the management of steelmaking by-products, such as slags, dust, and flue gases, can significantly affect the eco-profile of steel products, depending on the LCA modeling approach used for co-products [5].

From a methodological standpoint, mathematical optimization and LCA have already been applied in the steel sector. For example, Mixed Integer Linear Programming (MILP) has been used as a multi-criteria decision-making tool to evaluate trade-offs between various environmental, social, and economic indicators for steelmaking and aluminum production [6,7]. As an alternative optimization approach, some researchers have employed Data Envelopment Analysis (DEA) to identify correlations and maximize resource efficiency in processes [8]. Additionally, it emerged that optimization can effectively be used to improve the scheduling of foundry operations, thereby minimizing the environmental impact associated with electricity consumption [9,10]. However, to the best of our knowledge there is currently no study available that addresses the optimal mix of materials to minimize LCA indicators in the steel sector, even though similar models have been developed for the aluminum industry [11].

In this context, it emerges that managing the environmental impact of EAFs is a complex task, which requires the identification of the optimal mix of scrap and tapping additions to minimize the environmental footprint of steelmaking. Therefore, the aim of this paper is to propose a methodological discussion on the development of an optimization model for EAFs, which is currently being pursued under the framework of the European project 'ALCHIMIA - Data and Decentralized Artificial Intelligence for a Competitive and Green European Metallurgy Industry' [12]. This type of mathematical model is currently absent from the literature and will be developed using data from existing facilities owned by the ALCHIMIA partners [12].

2. Methodology

This section outlines the methodology we propose for developing an optimization model that calculates the optimal mix of scraps and ferroalloys to minimize the environmental burdens of a steelmaking process, i.e. what we define as an "Optimized LCA model". Our proposal is based on a previous methodological contribution analysing the implications of integrating LCA and optimization for decision-making in the context of prospective LCA [13], as well as on the ISO 14040 and ISO 14044 standards [14,15]. An approach similar to the one proposed here has already been successfully applied in the photovoltaics [16,17] and battery sectors [18].

The integration of LCA and mathematical optimization has been explored by various authors in the field of decision-making, also in the steel sector [6,7]. The consolidated approach to address decision-making issues within the LCA framework is based on scenario-based comparative LCA [13].

The scenario-based comparative LCA approach involves the comparison of multiple scenarios created by varying the parameters of the LCA model. For example, in the context of steelmaking plants, the design and comparison of alternative scenarios, e.g. with different input scrap composition, is needed to select the most environmentally sustainable option. In each scenario, the input and output flows are quantified during the Life Cycle Inventory (LCI) phase. Then, in the Life Cycle Impact Assessment (LCIA) phase, the inputs (of material and energy) and outputs (in terms of waste and emissions into air, water and soil) are translated into potential environmental impacts of each process and summed up to evaluate several LCIA impact categories of the product system under study [14,15]. The environmental impacts calculated during the LCIA phase are then compared to select the most environmentally sustainable scenario. The reliability of this approach depends heavily on the ability of LCA practitioners and process engineers to investigate all possible scenarios [13].

The Optimized LCA approach adapts the methodology outlined in the ISO standards [14,15] for integrating LCA with optimization. This approach involves the development of an algorithm in which the quantities of certain LCI flows are calculated to minimize the environmental impact of the process [13]. The rationale behind this approach is that the optimal scenario, i.e. the scenario with the lowest potential environmental impacts, may not be included among those evaluated in a scenario-based comparative LCA. Indeed, as the complexity of a model increases, an optimization model may identify complex solutions that are unpredictable in scenarios created "ex-ante". For instance, it has been shown that the optimal European mix for battery production and recycling to minimize greenhouse gas emissions is unexpected compared to existing scenarios available in the literature [16]. Similar considerations apply to the foundry sector, where various materials can be used in steel component production. However, it is important to note that the optimal scenario identified by an optimization model should still be validated by LCA practitioners [13].

Unlike scenario-based comparative LCA, where parameters are varied based on arbitrary assumptions, in this approach some model parameters are treated as variables in an optimization problem [13]. The setup details of the optimization problem described here are adapted from the ISO 14040 [13] and ISO 14044 [14] standards. The adaptations needed in each of the 4 phases of the LCA methodological framework to implement the "Optimized LCA model" are described in the following:

- *Goal and Scope Definition*: In the context of integrating optimization with LCA, this involves setting the objective function, which is the indicator that needs to be minimized, such as GWP or a single score environmental impact (after normalization and weighting). Additionally, the functional unit, reference output, system boundaries, and chosen LCIA method must be specified. The approach to end-of-life modeling should also be declared.
- *LCI:* During the LCI phase, all flows involved in the product system, such as emissions and resource consumption, are collected. The quantities of these flows can be classified as either (i) parameters or (ii) variables in the optimization problem. Parameters are assigned fixed values, and scenarios can be created to assess their variations. In this case, the optimization model shall be run for every scenario. Variables, however, are not assigned values during the LCI phase, as their quantities are determined by solving the optimization problem. The distinction between variables and parameters depends on the Goal and Scope of the analysis. For example, if the objective is to calculate the optimal mix of scraps and ferroalloys to minimize the GWP of steel production, these quantities are treated as variables, while other material quantities, such as the water used in the process, are fixed as parameters.
- *LCIA*: In the LCIA phase, the LCI data are converted into potential environmental impact indicators. In the proposed Optimized LCA approach, this calculation cannot occur directly, as the quantities have not been predetermined in the LCI phase. Instead, the LCIA is represented as a generic function dependent on the optimization variables. The objective function mirrors the LCIA phase, where the flow quantities (both parameters and variables) are multiplied by the unitary impacts of each flow, as determined by the selected LCIA method and impact category during the Goal and Scope definition phase. For instance, if silicomanganese is used and the goal is to minimize GWP, its unitary impact can be expressed as kg CO_2 eq per kg of silicomanganese. To ensure consistency with the functional unit definition (which is typically defined as the production of a certain mass of steel, e.g. 1 kg of steel), the overall impact is divided by the annual output flow (OF). A set of constraints is also typically required, such as mass and energy balances or other correlations linking parameters and variables for describing the chemical-physical process behavior. Once the optimization problem is defined in terms of variables, numerical parameters, objective and constraints, formulated problem is solved for identifying solutions that minimizes the objective function. Proper numerical algorithms, commonly adopted in mathematical programming to calculate the minimum of functions, are used for the scope
- *Interpretation*: the interpretation phase in Optimized LCA is crucial. Unlike scenario-based comparative LCA, where scenarios are designed by the LCA expert, in Optimized LCA, the optimal LCA results are generated by an algorithm. This complicates their interpretation, as the algorithm might suggest solutions that are unrealistic in real-world conditions. Therefore, interpreting the results might lead the LCA analyst to add new constraints to the model or revise certain assumptions.

Figure 1 provides a mathematical formulation of the proposed Optimized LCA approach. It outlines all the steps in the methodology, including examples relevant to steelmaking plant applications.

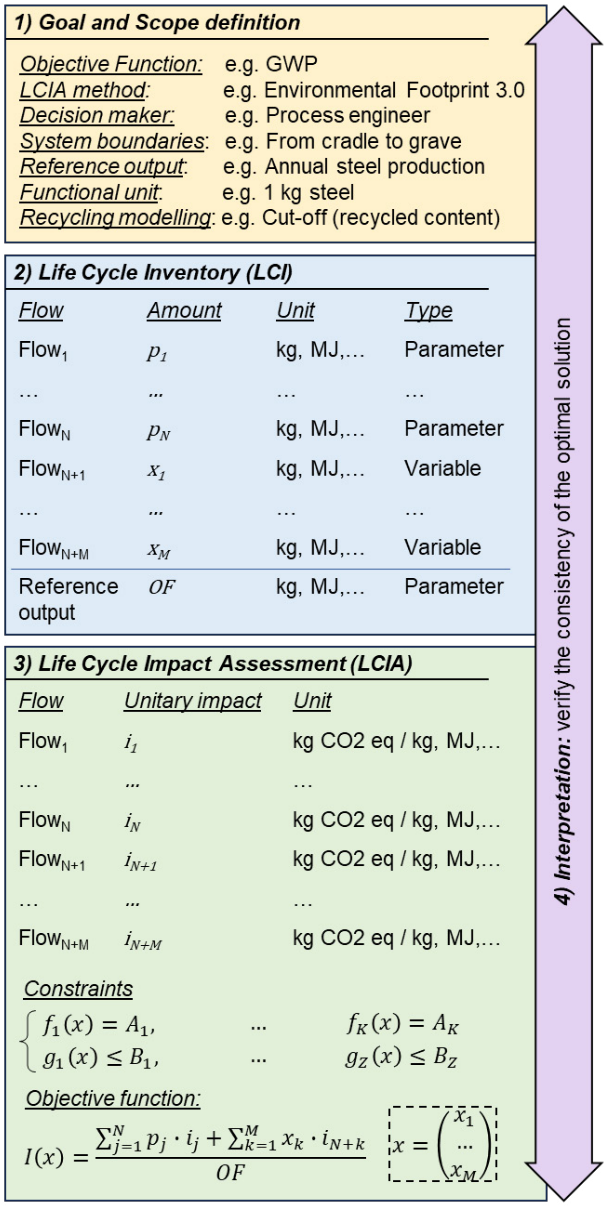

Fig. 1. Sketch of the Optimized LCA approach proposed here.

In Figure 1, parameter values are indicated as p whereas variables as x. The unitary impacts associated with the LCI flows are named as i. The number of parameters (excluding the reference output) is N while the number of variables is M. The number of unitary impacts is $N+M$ because the reference flow is not associated with any predetermined environmental impact value. Concerning the optimization constraints, K equality constraints and Z inequality constraints are set. In each constraint, functions f and g are constrained to be equal or less equal to A and B.

Concerning recycling modeling, practitioners can choose between several options for the LCA modeling of metals recycling that are available in literature [19,20]. The discussion around the most suitable recycling LCA modeling approach is outside the scope of this paper. However, it shall be highlighted that this choice affects the values of the unitary environmental impacts *i*. Hence, in case the choice of the recycling modeling is uncertain for the LCA practitioner, we recommend performing a sensitivity analysis to assess the variations of the Optimized LCA results depending on the selected modelling approach.

3. Case study

This section details the application of the Optimized LCA approach to a case study from the ALCHIMIA project [12]. The overall aim of the ALCHIMIA project is to develop methodologies for the environmental optimization of steelmaking processes through the application of digital technologies based on Artificial Intelligence techniques (https://alchimia-project.eu/). The project consortium includes several steelmaking companies, such as CELSA Group, which operates steel foundries in France, Spain, and Poland [21]. Within ALCHIMIA, a "traditional" LCA analysis will be conducted for the three CELSA sites mentioned above. Specifically, the results from the traditional LCA analysis will serve as a benchmark to assess the environmental benefits of the application of the Optimized LCA method to CELSA France. The case study description follows the steps of the Optimized LCA approach outlined in Figure 1.

3.1. Goal and Scope definition

The goal of this study is to address a decision-making problem: determining the optimal mix of steel scraps and ferroalloys that minimizes the environmental impacts of the steelmaking process. Several options are available for defining the objective function. One approach is to minimize one of the impact categories calculated by the LCIA method. The most significant impact categories for the metals sector are the following [22]:

- Global warming potential
- Acidification potential
- Eutrophication potential
- Smog potential
- Ozone depletion potential

Each of these five environmental indicators can be minimized individually and therefore five different solutions are obtained. Alternatively, to address all these indicators simultaneously, a new objective function can be established using a single score indicator (based on the normalization and weighting of the above-mentioned indicators). For this case study, the LCIA method selected is the method recommended by the European Commission Environmental Footprint 3.0 [19], given that ALCHIMIA is a European Project. The system under evaluation is a steelmaking plant owned by the CELSA Group and located in France [21].

As illustrated in Figure 2, the system boundaries of the study extend from cradle to gate. They encompass the EAF used for melting steel scraps and internal returns from the steelmaking plant, a crucible where various tapping additions (e.g., ferroalloys) are made, and a ladle furnace (LF) where other ferroalloys are added, Argon is used for stirring the hot metal to accelerate the chemical reactions and enhance the quality of the steel output, which is the output flow. The direct emissions are a mix of several substances, including fossil carbon dioxide, carbon monoxide, methane, particulate matter, SO_x, NO_x and other organic and inorganic compounds. An internal return of pre-consumer scraps is also considered as an input.

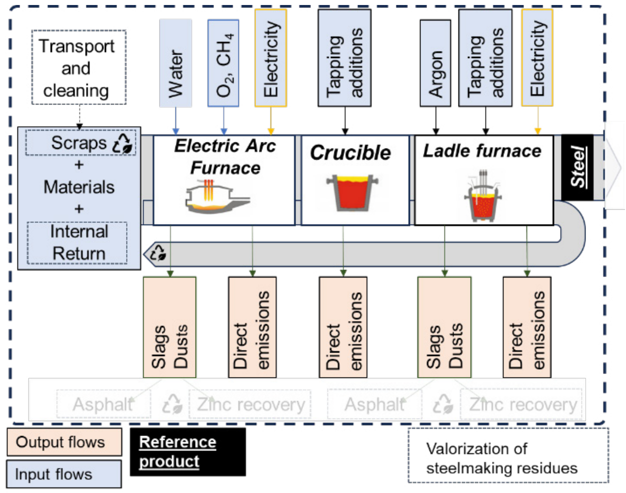

Fig. 2. System boundaries of the Life Cycle Assessment (LCA) for the CELSA France case study.

The functional unit is the production of 1 kg of output melted steel. The system boundaries also include the recovery of steelmaking residues such as slags and dust. The slags are recovered as an inert material in asphalt production, while the dust undergoes treatment for zinc recovery. Regarding the choice of recycling modelling, in this paper we follow the "cut-off" or "recycled content" approach [20]. The choice of this approach implies that the impact of secondary materials is null, and the recycling of wastes and co-products is not considered (neither the impact nor the environmental credits). However, as discussed in Section 2, a sensitivity analysis is recommended to assess the impact of the choice of the approach to model recycling on the optimization model's results.

3.2. Life Cycle Inventory and Life Cycle Impact Assessment

This section covers the LCI and LCIA phases of the Optimized LCA methodology application. The LCI is based on the Ecoinvent 3.8 (cut-off version) background database [23] and data from the scientific literature [24,25]. Table 1 lists the flows that constitute the LCI of the steelmaking process depicted in Figure 2. These flows include the consumption of materials and electricity, as well as the production of dust, slags, wastewater, and gaseous emissions. As mentioned in Section 2, some of these flows are treated as variables, while others are treated as parameters. Given that the study's goal is to calculate the optimal mix of scraps and ferroalloys, these flows are associated with the variables $x_1,\ldots,x_{16}$. Remarkably, in case the scenario-based comparative LCA approach is used instead of Optimized LCA, LCA practitioners would be required to create a very large number of scenarios to cover all the reasonable combinations of $x_1,...,x_{16}$. Electricity consumption is another variable in the optimization problem, as the amount of electricity consumed correlates with the types of metals melted in the EAF and LF. Excluding electricity and water, all variables and parameters are expressed in kilograms relative to the functional unit to facilitate mass balances.

Table 1. Summary of the LCI phase, including the distinction between parameters and variables, and of the LCIA phase, including the calculation of unitary environmental impacts (based on the Ecoinvent v3.8 database [23]).

Flow	Amount	Unit	Type	i	Unitary impact	Unit
Water	p_1	m^3	Parameter	i_1	0.45	kg CO2 eq/m^3
Slags	p_2	kg	Parameter	i_2	0.00	kg CO2 eq/kg
Dusts	p_3	kg	Parameter	i_3	0.00	kg CO2 eq/kg
Direct emissions	p_4	kg	Parameter	i_4	1.00	kg CO2 eq/kg
Wastewater	p_5	m^3	Parameter	i_5	0.17	kg CO2 eq/kg
Internal returns	p_6	kg	Parameter	i_6	0.00	kg CO2 eq/kg
Scraps	x_1	kg	Variable	i_7	0.06	kg CO2 eq/kg
Aluminum	x_2	kg	Variable	i_8	7.48	kg CO2 eq/kg
Ferroboron	x_3	kg	Variable	i_9	8.76	kg CO2 eq/kg
Ferrochromium	x_4	kg	Variable	i_{10}	5.17	kg CO2 eq/kg
Ferrosilicon	x_5	kg	Variable	i_{11}	6.81	kg CO2 eq/kg
Silicomanganese	x_6	kg	Variable	i_{12}	5.40	kg CO2 eq/kg
Titanium	x_7	kg	Variable	i_{13}	50.80	kg CO2 eq/kg
Vanadium	x_8	kg	Variable	i_{14}	28.90	kg CO2 eq/kg
Electricity	x_9	kWh	Variable	i_{15}	0.076	kgCO2eq/kWh
Anthracite	x_{10}	kg	Variable	i_{16}	0.47	kg CO2 eq/kg
Dolomite	x_{11}	kg	Variable	i_{17}	0.04	kg CO2 eq/kg
CaO	x_{12}	kg	Variable	i_{18}	0.02	kg CO2 eq/kg
Graphite	x_{13}	kg	Variable	i_{19}	0.02	kg CO2 eq/kg
Argon	x_{14}	kg	Variable	i_{20}	1.21	kg CO2 eq/kg
CaC_2	x_{15}	kg	Variable	i_{21}	3.51	kg CO2 eq/kg
CH_4	x_{16}	kg	Variable	i_{22}	0.53	kg CO2 eq/kg
Steel Production	OF	kg	Parameter			

The unitary impacts i presented in Table 1 were calculated based on the datasets summarized in Appendix A (Table 1A). Given that the cut-off approach was selected for recycling modelling, the unitary impact of recycled input materials is set to zero [19]. Consequently, the impact associated with scraps stems from sorting, pressing, cleaning, and transportation to the steelmaking site, while the impact of internal returns is null. Since slags and dusts are subject to recycling, the unitary impact their recovery is also zero according to the principles of the "cut-off" approach [20]. Some constraints are used to guarantee the reliability of the optimization model. For brevity, a summary of these constraints is provided below:

- *Mass Balance Constraints*: mass balance equations ensure that the total mass of inputs, such as steel scraps and ferroalloys, equals the total mass of outputs, including the final steel product and by-products like slags and dust as well as the emissions. For example, the total of the materials consumed ($x_{1,..,16}$) must be equal to the amount of steel produced (OF), the co-products and wastes ($p_{1,...,6}$).
- *Energy Balance Constraints*: the energy consumed during the steelmaking process, particularly in the EAF and LF, must be within operational limits. These constraints also account for energy efficiency, ensuring that the energy input is appropriately converted and used, with minimal losses. The energy balance is numerically described by first principle equations for the EAF and through artificial interlligence based model for the LF.
- *Material Quality Constraints*: To guarantee the quality of the final steel product, constraints are used on the composition of elements and contaminants, such as carbon and manganese, ensuring the steel meets specific standards. Such compositional assessment is based on specific numerical models have been developed for correlating: (i) the scrap composition and material additions with the final EAF steel composition; (ii) the starting steel composition and ferroalloys additions with the final LF steel composition. The specific EAF model is based on linear correlations tuned through real data, while LF model is based on neural network architecture. Correlations can also be used to assess the quality of co-products and evaluate possible advantages deriving from their recycling depending on the modelling approach.

4. Conclusions

In this paper we presented a methodological discussion on integrating LCA with mathematical optimization in the steelmaking industry. Specifically, we proposed the application of a methodology we defined as "Optimized LCA," inspired by existing literature and international standards, to a case study in France. The steelmaking site under evaluation is an EAF plant where steel scraps are melted together with ferroalloys and other materials. The Optimized LCA model aims to determine the optimal mix of scraps and ferroalloys to minimize the environmental impacts of the steelmaking process. This paper does not present results; instead, it focuses on the methodological discussion surrounding the model's variables and parameters, the definition of the objective function, the optimization constraints, and the influence of end-of-life modeling. Given the large variety of materials processed in EAFs, multiple scenarios would typically be required to evaluate all possibilities. Therefore, the primary advantage of Optimized LCA lies in its ability to reduce the effort required by LCA practitioners in calculating the optimal materials mix for EAFs, thereby minimizing the number of scenarios needed for a comprehensive evaluation. As a follow-up to this study, we will develop the Optimized LCA model in accordance with the methodological guidelines presented in this paper and quantify the environmental benefits of applying Optimized LCA compared to the traditional LCA model. Particular attention will be given to i) the selection of environmental impact indicators for defining the objective function, and ii) the valorization of steelmaking co-products using different LCA recycling modeling approaches. The output of ALCHIMIA will be a multi-objective optimization model that integrates Optimized LCA with an economic objective function. As a follow up of the methodological discussion presented here, the results of the study will be assessed. Moreover, a sensitivity analysis will be performed to assess the range of the optimization variables. An automated consistency check will be also implemented in the model to guarantee its reliability.

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Appendix A

Table 1A. Summary of the Ecoinvent v3.8 datasets used in this paper [23].

Flow	Dataset
Anthracite	"Hard coal {Europe, without Russia and Turkey}| hard coal mine operation and hard coal preparation"
Dolomite	"Dolomite {RER}| dolomite production"
CaO	"Lime {Europe without Switzerland}| lime production, milled, loose"
Graphite	"Graphite {RER}| graphite production"
Argon	"Argon, crude, liquid {RER}| air separation, cryogenic"
CaC_2	"Calcium carbide, technical grade {RER}| market for calcium carbide, technical grade"
CH_4	"Natural gas, high pressure {FR}| market for natural gas, high pressure"
Water	"Water, deionised {Europe without Switzerland}| market for water, deionised"
Direct emissions	Overall amount of gaseous pollutants (e.g. CO_2, SO_X, NO_X, particulate) released into the atmosphere. Extracted from "Steel, low-alloyed {Europe without Switzerland and Austria}| steel production, electric, low-alloyed".
Wastewater	"Wastewater from pig iron production {Europe without Switzerland}| market for wastewater from pig iron production"
Internal returns	Pre-consumer scraps that are recovered inside the steelmaking plant. "Iron scrap, unsorted {GLO}| iron scrap, unsorted, Recycled Content cut-off"
Scraps	Adapted from "Iron scrap, sorted, pressed {RER}| sorting and pressing of iron scrap" including transports and pre-treatments.
Aluminum	"Aluminium, primary, ingot {IAI Area, EU27 & EFTA}| aluminium production, primary, ingot"
Ferroboron	Adapted from "Ferronickel {GLO}| ferronickel production" changing the material composition
Ferrochromium	"Ferrochromium, high-carbon, 68% Cr {GLO}| market for ferrochromium, high-carbon, 68% Cr"
Ferrosilicon	"Ferrosilicon {RoW}| ferrosilicon production"
Silicomanganese	Adapted from [23]
Titanium	"Titanium {GLO}| titanium production"
Vanadium	Adapted from [24]
Electricity	"Electricity, high voltage {FR}| market for electricity, high voltage "

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