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A comprehensive design approach to increase the performance of steels under minimal costs and environmental impacts

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ABSTRACT

The requirements for new materials are increasing, as multidimensional criteria should be included in the material design process. A comprehensive approach for designing new steels is presented, where the environmental dimension for each alloying element is considered, besides the technological and economic aspects. A case study focuses on increasing the hardenability of air-hardening steel. Economic and environmental figures expand the technical perspective. It is demonstrated within this study that standard alloying elements used to increase the hardenability significantly influence further selection criteria. It is exemplified that alloying elements like boron provide higher hardenability at lower costs and a lower carbon footprint than, for example, nickel or chromium. This comprehensive design approach can be transferred to other technological optimization phenomena. It might help design future generations of steel by considering further objectives and disclosing possible trade-offs.

1. Introduction

Steel is the backbone of modern infrastructure. Because of its versatile properties, steel is used as a structural material in various applications, from reinforced bars for building bridges, over rails to forged components for chassis and drive trains in the automotive industry [1,2]. An ongoing effort exists to develop and optimize existing and new steel grades. The alloying concept is crucial for achieving specific properties, which are determined by the target functions of the application. For most steel forgings, the steel must have high strength and ductility to deal with mechanical loads. Typical steel components which are produced by forging are axle journals, crank shafts, rotor shafts and planet carriers. Usually quenching and tempering (Q + T) steels are used for these applications, which are characterized by a three-step heat treatment after forging consisting of austenitization, quenching, and tempering. These Q + T steels have a martensitic microstructure [3] (carbon supersaturated α-iron [4]) with small carbon precipitates equally distributed in the martensitic matrix. The mechanical properties of these steels show generally high strength and good impact toughness values in the Q + T condition combined with a high surface hardness. The martensitic phase transformation needs high cooling rates to prevent other diffusion-controlled phase transformations, so the thickness of forged components made from Q + T steels is limited. Q + T-steels are classically alloyed with 0.2 wt% to 0.6 wt% carbon [2], while additions of manganese [5] and chromium [2,6,7] as well as molybdenum [2,8] and nickel [2,6] are applied to increase the hardenability and impact toughness, respectively.

Most recently, a new type of air-hardening high-strength steel was developed on the laboratory scale [9,10] and successfully produced in an industrial trial [11,12]. Contrary to previous steel concepts, these steels achieved a martensitic microstructure without quenching simply through air-cooling, as the alloying concept suppresses other phase transformations. These air-hardening ductile (AHD) forging steels have a comparable high hardenability, achieved by a significant addition of approximately 4 wt% manganese. Other elements are added to either influence precipitation processes (silicon [6,13], aluminum [14–16], and niobium [17]) or to tailor the transformation kinetics to specific component requirements (aluminum [18], molybdenum [19] and boron [20]). Caused by the goal to address primarily the needs of automotive suppliers with this steel grade, the focus was laid on relatively thin wall thickness, and the cost-intensive alloying elements chromium and nickel were not considered. Especially for large components like planet carriers for the mining industry, further modifications of the composition need to be made to achieve the necessary hardenability.

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While achieving specific material properties is the main target in material development, the design process is influenced by further motivations. As the steel is designed for industrial applications, the developed steel must be economically competitive compared to existing ones. The costs must be evaluated and monitored. Especially products in the automotive industry are often designed as a compromise between costs and properties [21]. Since the beginning of steel development for automotive applications, these alloying-specific costs have mainly been related to raw materials and energy input. Substituting alloying elements with other, less expensive elements is theoretically possible, but as the influence of the substituted element is versatile, some drawbacks are introduced. For example, the standard quench and tempering steel 42CrMo4 (AISI4140) is alloyed with chromium and molybdenum, both costly elements. Attempts were made to substitute molybdenum with manganese [22], and chromium with manganese [23], as manganese is a relatively cheap alloying element [2], but the resulting steels (42MnCr4–4; 45Mn8) had inferior mechanical properties. This substitution effort illustrates possible trade-offs between the technical and economic dimensions. Next to the technical and economic dimension, the societal perspective gains attention, and the environmental burden is more often considered [24,25]. Environmental criteria are not only linked to social responsibility and are thus reflected in the corporate reputation. The increasing pressure to act also results in political instruments such as CO_2 pricing, which has an increasing influence on the steel industry in terms of costs. Against this background, indicators such as the carbon footprint must be considered in developing steel as it has economic and environmental consequences. The calculation of the carbon footprint of steel components is a complex process, as raw materials, steel production, processing, and heat treatments contribute to changing quantities in the overall footprint [26,27]. While the costs of alloying elements are often well-known and already considered within the community of steel-developing engineers and scientists, the environmental impact of the production of the alloying elements is often overlooked. Additionally, further indicators of the environmental dimension can be relevant for the material development process and its usage in industry. For example, energy demand is of growing importance due to geopolitical tensions. The same applies to resource availability, which is often discussed in the context of alloying elements.

This study aims to introduce a methodological approach to include various decisive factors in alloy development regarding aimed material characteristics with the example of hardenability. It should guide engineers in finding solutions when considering multiple decision factors in material development processes. Therefore, the research questions addressed in this article are:

(i) How can the content of alloying elements achieve a defined technical requirement as hardenability be calculated?
(ii) How can further dimensions relevant to the choice of alloying elements, such as the environmental and economic perspective, be integrated?
(iii) How does considering multiple dimensions influence the choice of alloying elements?

The study will first give an overview of the alloy design process regarding the technical requirement of hardenability. The discussion and calculation of parameters of the economic and environmental dimension follow it. The change in technical, economic, and environmental parameters and their relation is then illustrated by a case study of a forged component. By comparing the impacts on the comprehensive performance of a material, new insights for sustainable steel design can be received. The present study aims to guide engineers and scientists in practice on finding sustainable solutions when the requirements of an alloy design change and multiple decision factors must be considered. Contrary to the current industrial and scientific approaches, where mostly only the technical goal is considered and the associated costs are considered, we are investigating a framework which alloys to design of new steels based also on different environmental impacts. This approach will allow users to base their decision not only on economic but also on ecological aspects.

2. Method

The optimization of steel products is a process that is significantly influenced by the respective goals of the manufacturing company as well as the political, economic, and ecological boundary conditions. At the technological level, the optimization process can be simplified as a flow chart, starting with the initial product and ending with the optimized product, see Fig. 1.

A property with optimization potential is first identified at the beginning of the optimization process. In the next step, the necessary parameters are determined to optimize this property, and target values for the parameters are set. It must be stated at this point that a change of chemical the chemical composition has always mutual influence on the performance of a material. However, to demonstrate the importance of a comprehensive design approach, the case study was simplified to only cover the effect of hardenability. Therefore, the material properties are always related to the target function of applications. The next step is the actual optimization, which, for most common steel products, can be divided into optimization concerning component geometry, process optimization, and adaptation of the alloy. These different optimization approaches are often activated simultaneously as the changes influence each other. In the case of material optimization, new compositions are then determined to fulfill the boundary conditions. The specific product is first determined to determine a specific change in the material property. After the parameters and target values have been determined, the optimization of the material can be regarded as independent of the product since only the relative change in a material property is to be determined. Among the possible alloys, the alloy that meets the target values and the boundary conditions is selected based on defined criteria. Up to now, the most important criteria have been changes in production costs. In the context of sustainable production, however, this is no longer appropriate since criteria such as changes in the carbon footprint and the cumulative energy demand must also be considered. Carefully considering as many boundary conditions as possible guarantees comprehensive material optimization in this context. In the following, this approach is presented using the example of a forged steel product. The component was produced on the industrial scale via ingot casting. The melt (40 t) was cast in 12 conical ingots of 3.3 tons each, with a diameter of 420 to 520 mm and a length of 1960 mm followed by pre-blocking to 245 mm square. Prior to the forging, austenization was performed at 1250 °C, followed by pre-compressing and then forged in several strokes. The components were then deposited for air hardening. The temperatures of the blanks and components were recorded with a pyrometer during forging.

2.1. Determination of necessary alloying additions

Recently, new materials for the forging industry have been developed that achieve their final properties through air-cooling, omitting a cost, and CO_2-emissions intensive heat treatment (austenization, quenching, and tempering). These steels are alloyed with different elements to control the phase transformation and especially prevent the formation of the bainite phase. The chemical composition of a recently introduced air-hardening forging steel is displayed in Table 1. The chromium and nickel concentrations are not alloyed intentionally but originate from impurities of other input materials. The steel has been industrially produced by ingot casting (charge weight 50 t; ingot weight 3.3 t) and was subsequently pre-blocked. Bainite formation was still observed for large forging components with thick diameters, as the heat transfer is not fast enough to reach the critical cooling velocity for bainite suppression. An exemplary component produced from this steel is a planet carrier (about 226 kg). Fig. 2 displays this steel's continuous

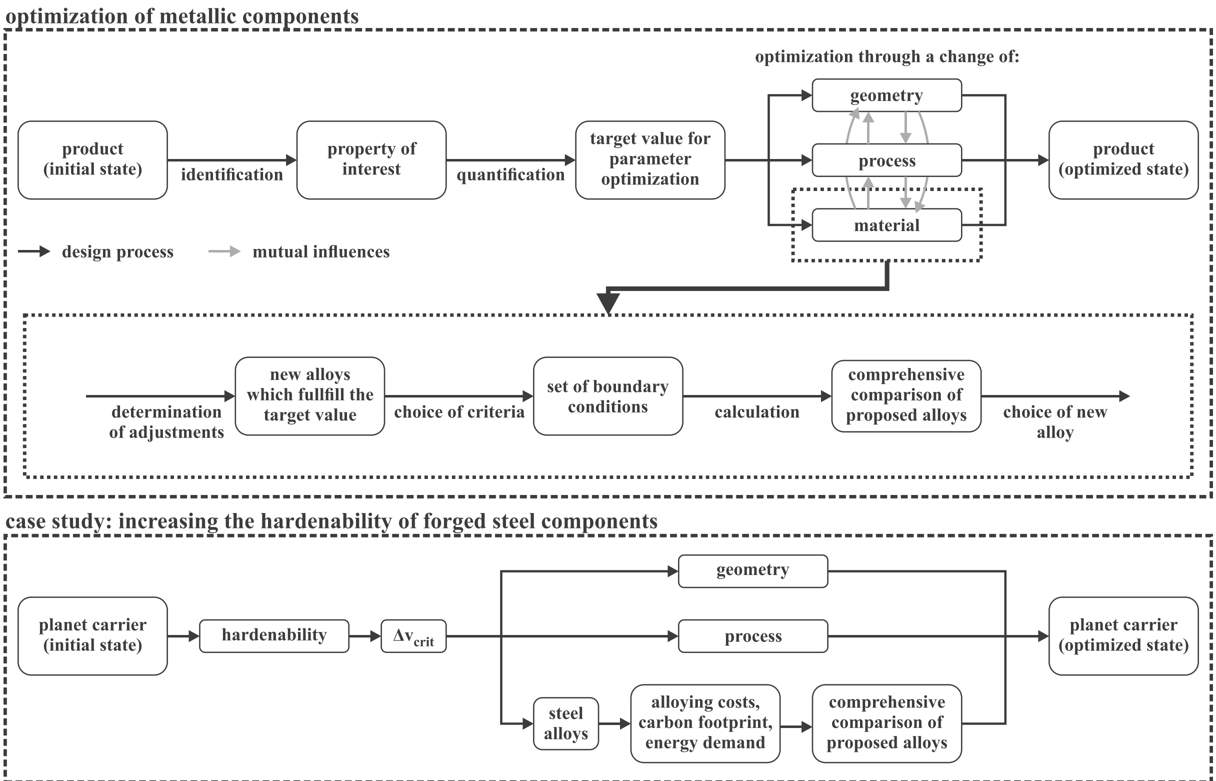

Fig. 1. Simplified flowchart of the optimization process for metallic components. The design process from the initial to the optimized product state is displayed. Generally, an optimization can be done by changing the geometry, the production process, or the material of a steel component. In this case, emphasis is placed on the material. Additionally, the application to the present case study is displayed. The critical parameter, hardenability, must be adjusted to reach the required mechanical properties. The change of the critical cooling rate Δv_{crit} needs to be reached by modifying the chemical composition, which results in new steel alloys. Based on specific boundary conditions (e.g., alloying cost, carbon footprint, energy demand), a comprehensive comparison can lead to a new chemical composition and, finally, the optimized state of the product.

Table 1
Chemical compositions of the investigated air hardening ductile (AHD) forging steel determined by spark spectral analysis. All concentrations are given in wt.-%.

Fe	C	Si	Mn	Cr	Ni	Mo	Al	Nb	B
Balance	0.15	0.50	3.90	0.10*	0.10*	0.24	0.52	0.03	0.0025

cooling transformation diagram (CCT) with the measured cooling curves of the forged planet carrier.

CCT diagrams display the resulting phase fractions after a cooling schedule. Additionally, an engineering drawing of the component is added to the diagram. As seen, the cooling curves hit the bainitic phase field, resulting in a mixed microstructure of bainite and martensite, which is unfavorable for the mechanical properties.

The optimization aims to achieve a fully martensitic microstructure by accelerated cooling or adjusting the chemical composition, shifting the bainite formation to slower cooling rates. However, the control of the hardenability is not trivial, and the interactions of several elements (and their impact on CO_2 emissions and costs) need to be considered. Some empirical formulae are used in the literature to calculate the critical cooling rate from chemical composition. The natural logarithm of the critical cooling rate can be expressed by the sum of the elemental concentrations multiplied by a weighting factor and a parameter k_0, as displayed in Eq. (1):

$$ln(v_c) = k_0 + \sum_i k_i w_i \quad (1)$$

Eq. (2) was recently published and covers a wide range of materials [28]:

$$ln(v_c) = 16 - 4.62w_C - 1.70w_{Mn} - 4.00w_{Al} - 0.50w_{Cr} - 6.00w_{Mo} - 0.54w_{Ni} - 550\, w_B \quad (2)$$

The empirical formula describes the increase of a single alloying element needed to meet the new target values. An exemplary calculation for the necessary increase of chromium is displayed in the additional information. Besides using empirical formula, neural networks or machine learning (ML) algorithms can be used to predict the optimal changes to a specific alloy composition, as published by Vannucci et al. [29] or Allen et al. [30]. While these general approaches are of special interest for slight modifications of existing alloys (due to the large availability of data) for prediction of modifications which are out of the range of data which was used for training the dataset, the algorithm might not produce reliable results. Furthermore, boundary conditions need to be set appropriately. This is also true for empirical formula, however Eq. (2) was developed on a set of alloys similar to the steel in this study. The algorithm used by Allen et al. suggests the reduction of tungsten and cobalt in the investigated steel to 0, which will lead to notable cost savings. However, as these elements were not alloyed on purpose but are residual elements presumable from scrap, this solution is not feasible.

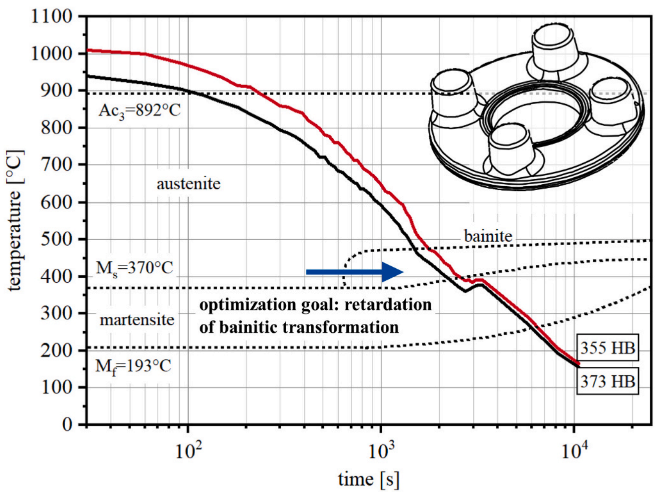

Fig. 2. Continuous cooling transformation (CCT) diagram of an air-hardening steel with the cooling curves of a forged planet carrier. The different curves visualize the influence of the component thickness on the local cooling rate. The black curve was measured in the disc of the component, while the red curve was measured in the stud. The cooling curves must reach the martensite start temperature (M_s) without crossing the bainite transformation area to achieve a complete martensitic microstructure. Different hardness values (HB: hardness measured by the Brinell method) were obtained and indicated at the end of the respective curve.

2.2. Economic impact of alloying elements

The cost drivers for large steel components like bearings are alloying elements, hot deformability, heat treatment, and carburization [31]. Elements like chromium, manganese, or molybdenum are added in steel production as ferroalloys (chemical compounds mainly containing the respective alloying element and iron). However, the concentration of alloying elements within the ferroalloys varies significantly. Ferrochromium, for example, is standardized into 5 groups by the chromium range with 45 wt% to 55 wt% chromium at the lower and 85 wt% to 95 wt% chromium at the upper end [32]. Further subdivisions are made based on carbon, silicon, phosphorus, and sulfur concentrations. In general, it can be assumed that the price increases with the content of the alloying element and purity, as an additional purification process will increase the production cost. Some applications require using electrolytically refined raw materials with even higher costs (and drastically increased CO_2 emissions [33]), as impurities are critical to the application. Conversely, for boron, the concentration in ferroboron ranges only from 10 wt% to 20 wt% [34]. Just et al. [35] tried in the past to quantify the costs of different steel grades, which resulted in the following regression analysis equation for steel bars:

$$Prize\left(\frac{DM}{kg}\right) = 0.51V + 0.56Mo + 0.30Al + 0.21Ni + 0.09Si + 0.08Cr + 0.03Mn + 0.82 \quad (3)$$

Fig. 3 exemplary displays the price fluctuations of four ferroalloys between 2013 and 2022. If the deviation for each element from its average prize of the displayed period are calculated, it can be seen that over a period of ten years the prizes of the elements peaked with increases of 111%, 69%, 52%, and 32% for ferro chromium, ferro molybdenum, ferro silicium and ferro tungsten, respectively. However, the approach leads to a prize ranking for different alloying elements, which is not based on the raw material (ferroalloys) prize but on a regression analysis of the final steel product. If this ranking is further compared with the influence on mechanical properties like hardenability, manganese and chromium achieve comparable high hardenability in

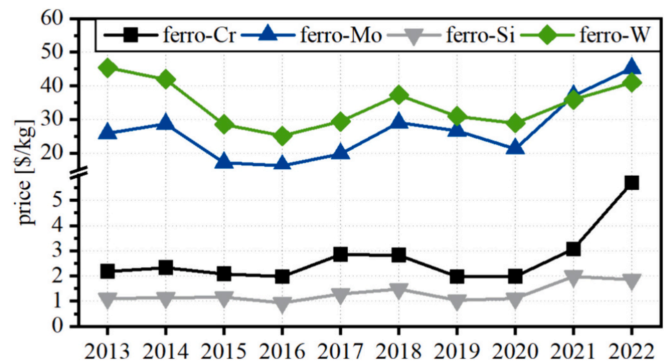

Fig. 3. Average global price of ferrochromium, ferromolybdenum, ferrosilicon, and ferrotungsten from 2013 to 2022 [36].

correspondence to the prize of the steel [35]. Those analyses are problematic today due to legal frameworks implemented to prevent cartelization.

Estimating the costs of changing the chemical composition is a complex problem, as changes not only influence the amount of necessary ferroalloys for steel production. Due to the higher needs of a specific ferroalloy, it might be necessary to change to a higher quality grade as the standard quality might include tramp elements to such an extent that large amounts of this ferroalloy will contaminate the whole melt. Sometimes, it is even necessary to change to electrolytically refined alloying elements. However, for a first estimation of the cost-increase, it was assumed that the cost increases linearly with the concentration of an alloying element, leading to the following equation of a rough estimation of the Δcosts for a forging component of weight m,

$$\Delta\text{costs} = \text{m} \bullet \Delta w_i \bullet t_{Fe-M} \bullet P_{Fe-M} \quad (4)$$

where $t_{Fe\text{-}M}$ and $P_{Fe\text{-}M}$ are the yield factor and the prize of the ferroalloys, respectively. The yield factor can be expressed as the reciprocal of $c_{Fe\text{-}M}$ multiplied by a factor t_{plant}, which represents the efficiency of the steel production process of a specific plant. As no information on this efficiency is available, the factor was set to 1 in the present study.

$$t_{Fe-M} = \frac{1}{c_{Fe-M}} \bullet t_{plant} \quad (5)$$

2.3. Environmental impact by alloying elements

The environmental impact calculation is based on the methodology Life Cycle Assessment (LCA), defined in the standards ISO 14040/44 [37–40]. An environmental LCA includes a variety of impact categories, such as acidification, climate change, eutrophication, and ecotoxicity. LCA follows the idea of life cycle thinking; therefore, a system should be covered holistically. However, material design processes are often in an early stage of a product development stage. Therefore, the final applications are not always clearly defined, and therefore, balancing an entire product system is often impossible or only with very high uncertainties. We use the environmental impact per kg alloying element, including all upstream processes, to estimate the effect on a material's environmental performance. The environmental impact per kg provides material scientists with a first approximation of the environmental effect on the material level. Also, it allows an alloy-specific assessment of the material produced. Metals are often considered one material flow in the environmental assessment, focusing only on the main metal, e.g., aluminum, iron, and copper [25,41,42]. The fact that the flows are interconnected and the material flows are even more complex is known [43] and applies to the material flow analysis and the LCA. It is also known that the impacts per kg of alloying elements are higher than those of the main metals [44]. Therefore, even though the focus is often on the main metal, the alloying elements are essential. Consequently, this study focuses on the varying input of alloying elements.

The covered impact categories are taken from the category framework ReCiPe 2016. While all impacts were calculated, the discussion and presentation focus on the Global Warming Potential (GWP), freshwater toxicity, human carcinogenic toxicity, and water consumption based on hotspots in metal production in the literature [45]. The GWP has an additional meaning as it is a direct link to the overarching goals at the policy level, where greenhouse gas (GHG) emissions, i.e., climate change, are in focus. Two additional indicators not included in ReCiPe were calculated: the material footprint (MF) and cumulative energy demand (CED). The MF was included to quantify the raw material required to realize the changed alloying composition [46]. The CED follows the same calculation but quantifies the energy required. The impacts per kg of alloying element were calculated using the LCA software OpenLCA (version 1.11.0) in combination with the ecoinvent database (version 3.9.1) [47,48].

Those impact factors per kg alloying elements were then brought together to calculate the delta caused by the possible changes in alloying concepts. The calculations are limited to that scope as the upstream processes regarding steel production remain unchanged and, at the same time, have high uncertainties as little information is available. By multiplying data representing the changes of alloying concentrations required [weight-percentage wt-% (Table 2) and the ore grade], the required amounts of alloying elements per element and change (delta) were calculated. Multiplying these required amounts with the environmental impact per kg of the alloying elements used and the preceding processes results in the additional environmental impact per kg AHD-steel.

3. Results

In the following chapter, the proposed framework will be performed exemplarily on a forged planet carrier, produced with a recently developed steel grate. The aim of this theoretical consideration is to assess the different alloying options for increasing the hardenability of the newly developed alloy, not only considering technological boundaries, but also economic and ecological ones. For this matter the necessary additions of hardenability increasing elements will be determined (Chapter 3.1), followed by the estimation of associated additional alloying costs (Chapter 3.2). Finally, the additional environmental impact, caused by supplementary alloying elements will be determined by LCA (Chapter 3.3).

3.1. Adjustments to the alloying concept

With the described approach, the necessary adjustments for each element (Δw) can be calculated. To achieve the desired hardenability, 0.45 wt% Cr, 0.13 wt% Mn, 0.41 wt% Ni, 0.04 wt% Mo or 0.0004 wt% B must be added to the initial steel composition. With the changes of the concentration, the additional amounts of alloying elements (Δi) (and their respective ferroalloys), the resulting alloying costs (Δcosts), and CO_2 emissions can be calculated. The resulting values for each alloying element are summarized in Table 2.

Table 2
Required changes in alloying concentrations to decrease v_c and the resulting increases in costs and CO_2 emissions. Additionally, the concentration of the ferroalloys ($c_{Fe\text{-}M}$). For the ferroalloys of Cr, Mn, Mo, electrolytic nickel [49–51], and ferroboron [52], the average market price from 2015 to 2020 is used.

	unit	Cr	Mn	Ni*	Mo	B
Δw_i	wt%	0.45	0.13	0.41	0.04	0.0004
Δi	kg	1.01	0.30	0.93	0.08	0.001
$c_{Fe\text{-}M}$ [49–51]	wt%	66	75	100*	75	18
ΔFe-alloys	kg	1.68	0.40	0.93	0.11	0.005
prize	$/kg	2.28	0.96	12.10	21.65	37.88
Δcosts	$	3.84	0.38	11.30	2.43	0.01
ΔCO_2-eq	kg	3.04–8.12	0.52	40.5	9.17	0.01

* Only data for electrolytically refined nickel was available from the available database.

The case study shows that the alloying elements used to increase hardenability have different specific costs and CO_2 emissions (Table 2). Boron and manganese are particularly advantageous for the optimization objective, whereas molybdenum, nickel, and chromium are questionable due to their high costs and carbon emissions.

3.2. Estimation of alloying cost increase

The resulting cost increases for a specific element, calculated by this method, are displayed in Table 2. As displayed, the costs of utilizing an alloying element for the optimization goal differ strongly in the dependency on the chosen element. Based on assumptions mentioned above and simplifications, choosing boron would lead to an overall cost increase of the component by only 0.01 $; manganese, molybdenum, and chromium to an increase of 0.381 $, 2.43 $, and 3.84 $, respectively. Using nickel would lead to a cost increase of 11.30 $, approximately three magnitudes higher than the increase caused by boron.

3.3. Environmental impact

By multiplying data representing the changes of alloying concentrations required (in wt%, Table 2) and the ore grade [12], the required amounts of alloying elements per element and change (delta) were calculated. Multiplying these required amounts with the environmental impact per kg of the alloying elements used and the preceding processes results in the additional environmental impact per kg AHD-steel. The relevant factors are *freshwater ecotoxicity* [kg 1,4-DCB], *global warming potential (GWP)* [kg CO_2 eq], *human carcinogenic toxicity* [kg 1,4-DCB], *water consumption* [m^3], *cumulative energy demand (CED)* [MJ-eq] and *total material requirement (TMR)* [kg]. Per kg alloying element, the impact of molybdenum (Mo) is the most significant regarding freshwater ecotoxicity, GWP, water consumption, CED, and MF. Only when it comes to human carcinogenic toxicity the impact of ferromanganese (Mn) is the most significant.

By multiplying the required amounts of alloying elements per element and changing with the environmental impacts per kg alloying element, it turns out that throughout all six impact categories, boric acid (B) has the least significant impact, which is due to the low impact per kg in general, but also to the low amount of material needed (only 0,02188 g). It is noticeable that for freshwater ecotoxicity and MF, molybdenum (Mo) still has the most significant impact, and for human carcinogenic toxicity, ferromanganese (Mn) still has the most significant impact. However, due to the low concentration of Nickel (Ni 6,25), a relatively high input is required, resulting in the environmental impact of Ni 6,25 being the most relevant regarding GWP, water consumption, and CED.

However, these results might vary depending on the origin of the alloying element. A comparison of different source from the literature reveals that the effect of chromium on the GWP might vary from 1.6 to 7.2 [kg CO_2 eq/ kg]. An overview of the data variation is displayed in Table 5 in the appendix.

4. Discussion

The state of the art of alloy design in the steel industry is based on two main boundary conditions: (1) achieving the technological goal and (2) the additional costs for changing the alloying elements. In our work we propose to include environmental impacts already at the design state, to prevent long and costly development processes which will end up with a less sustainable product. In the long term, the proposed framework can be included into integrated computational materials engineering (ICME) approaches, to design new steels and other materials based on their environmental impact. In the following chapter, the results obtained by our assessment of different alloying possibilities will be discussed (Chapter 4.1.1–4.1.3) and from the results obtained a, in our opinion, best alloying strategy for increasing the hardenability will be chosen (Chapter 4.1.4). The section is followed by a critical assessment of the limitations of our LCA approach (Chapter 4.2.) and finally by a general critical assessment of our proposed framework.

4.1. Comprehensive optimization

Centered on the results displayed in Table 2 and Table 3, an alloying element for increasing the hardenability of the investigated forging component can be chosen, considering technological, economic, and ecological aspects.

4.1.1. Technical perspective

From the technological point of view, calculated composition adjustments would be possible for all elements, as all additions are relatively low and, therefore, feasible. None of the elements is known to cause problems during production within the respective range. The increases of molybdenum and boron are barely notable. However, it can be assumed that from a technological and metallurgical perspective, smaller changes to the alloy are more favorable as different process-relevant parameters like liquidus- and solidus-temperature are less influenced. Especially the flowability of steel melts is of key interest for steel producers at it is widely known that changes of the composition will result in different viscosity of the melt [53,54] and the slags [55]. For the presented alloy the addition of manganese and aluminum can be considered most critical, as especially in combination these elements reduce the hot ductility during continuous casting [56]. From a technical perspective, it can be stated that adding 0.0004 wt% boron will have fewer secondary effects than adding 0.41 wt% nickel. Due to the very precise but necessary adjustment of 4 ppm boron, the question arises if manufacturers can implement this modification, but as producers of boron alloyed steels mostly work in the range of 25–60 ppm boron, this modification can be considered possible.

4.1.2. Economic perspective

A comparison of the associated price increases explains the reservations of the automotive industry against nickel and chromium, as nickel is by far the most expensive option, and chromium is still approximately 60% more expensive than molybdenum. Manganese and boron are, therefore, most favorable from the economic point of view, as the additions lead to barely notable cost increases of the component (of 0.38 $ and 0.01 $, respectively). Molybdenum results in +2.43 $ per component, which seems tolerable compared to the other elements. The economic influence was considered in the case study for simplicity reasons with one steady price. However, numerous influencing factors exist, such as the price development of ore, transportation, carbon emission, scrap, policies, and varying supply and demand. This results in volatile prices highly influenced by the market and economic situation [57]. The same applies to the price development of alloying elements, which is clearly shown by the price development, especially during the pandemic crisis. The prices of alloying elements were stable from 2011 until 2015, followed by low prices and heterogenic price development. The latter resulted, on average, in increasing prices. At the beginning of the pandemic in 2020, prices were decreasing on average, but the price development varied substantially between ferromolybdenum (−19%), ferromanganese (−14,9%), ferrochromium (+0,3%), and iron ore (+15,9%) [51]. China enormously influences the steel market due to being the largest steel producer and consumer [51,57]. In the future, the price volatility of alloying elements should be included.

Table 3
Comparison of different environmental impact categories. The best (lowest impact) and worst (highest impact) alloying elements are listed for each assessed category. It is differentiated between the impact of the alloy element itself and the impact caused by the specific amount (compare Table 2) needed to achieve the required properties. The two perspectives might vary as different amounts must be added for each element.

Impact category	Lowest impact per kg alloying element	Lowest impact per kg AHD steel	Highest impact per kg alloying element	Highest impact per kg AHD steel
Freshwater ecotoxicity **[kg 1,4-DCB]**	Cr 68%	B: **6.88×10^{-6}**	Mo	Mo: **0.066**
Global Warming **[kg CO_2 eq]**	B	B: **3.326×10^{-6}**	Mo	Ni 6,25: **0.224**
Human carcinogenic toxicity **[kg DCB eq]**	B	B: **3.33×10^{-6}**	Mn	Mn: **0.135**
Water consumption **[m^3]**	Mn	B: **3.326×10^{-6}**	Mo	Ni 6,25: **1.424×10^{-3}**
CED **[MJ-eq]**	B	B: **0.365×10^{-3}**	Mo	Ni 6,25: **3.432**
TMR **[kg]**	Cr 68%	B: **0.689×10^{-3}**	Mo	Mo: **2.826**

4.1.3. Environmental perspective

The third criterion considered is the environmental impact. As displayed in Table 2, small amounts of molybdenum already cause the highest environmental impact, which is at least comparable to the amount caused by the tenfold chromium content. When deciding between alloying with chromium or molybdenum, it can be said that from an economic perspective, molybdenum should be favored, but the ecological perspective favors chromium. The other elements stay in the same ranking order, with boron being the most favorable element, followed by manganese. Nickel has by far the highest emissions, but as mentioned before, this is partly caused by the fact that the data for electrolytic nickel was used.

4.1.4. Merging of the perspectives

In our example, the ‘set of boundary conditions’ (compare Fig. 1) are alloying costs, carbon footprint, and energy demand. The comparison of all conditions leads to the decision that boron is the element of the choice, leading to an optimized product. Relative to traditional production methodologies, one could assert that the optimization strategy embodies a reversed process chain. The comprehensive approach commences with the product, subsequently identifies and analyzes the requisite process and material parameters, and ultimately culminates in determining an optimal material composition. A visualization of this comparison is displayed in Fig. 4. The best option is represented by the center of the radar diagram, and the worst by the periphery. The closer the elements are positioned to the center, the better their ranking is. Boron should be used to optimize the hardenability, as the change is technologically possible, has the lowest costs, and the lowest environmental impact. In addition to the CO_2-eq, additional environmental indicators have been assessed and compared. These factors were then merged to enable a more comprehensive comparison of the environmental effects. When the environmental assessment is not limited to the CO_2-eq (GWP), manganese surpasses chromium, mainly caused by the relatively high human carcinogenic toxicity.

So far, the merged environmental indicator was calculated by weighting each indicator equally. In the future, the different environmental indicators could be weighted based on specific boundary conditions of production. For example, if the production of the respective steel component takes place in a humid region, the water consumption factor could be less relevant.

4.2. Comments on the environmental impact

When it comes to the scope of the environmental analysis, it is crucial to recognize the reach of the implications derived from the analysis. It

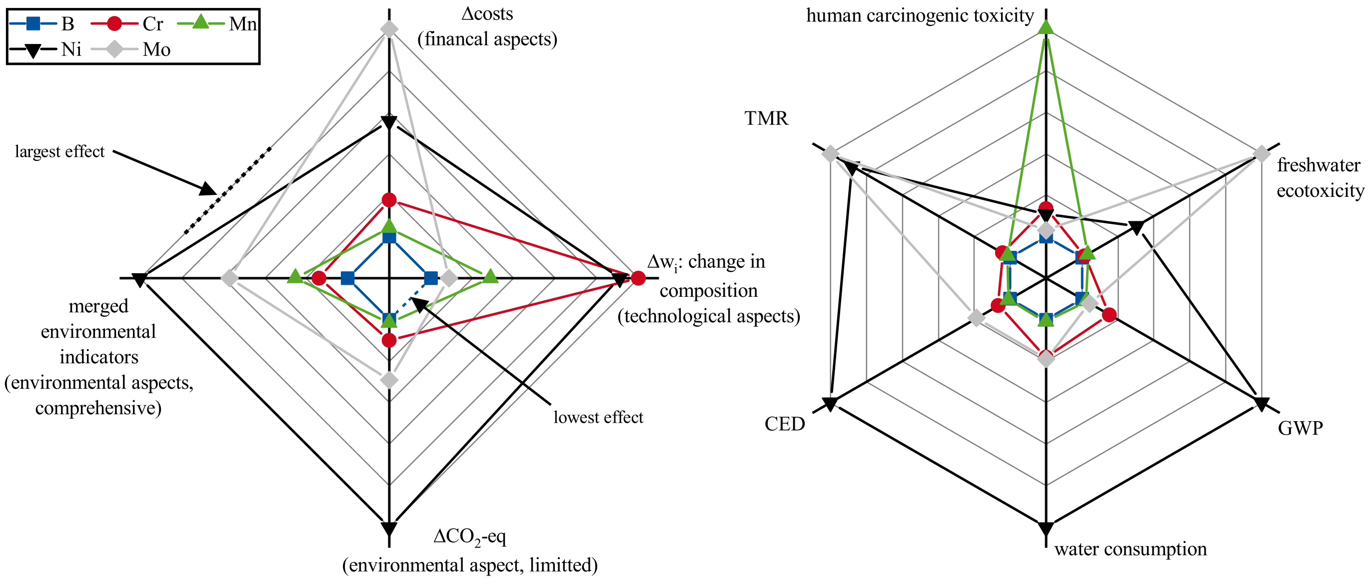

Fig. 4. Visualization of the comprehensive comparison of different alloying elements. The left diagram displays the necessary change in chemical composition (Δw), the increase in alloying costs (Δcosts), and the increase of the CO2-eq, which are caused by the investigated elements chromium, manganese, nickel, molybdenum, and boron. B. Further environmental indicators are plotted and merged into a new factor, enabling a comprehensive environmental comparison.

supports quantifying the influence of the choice of alloying concept on the environmental impact on the material level. This way, the environmental perspective can be included in material design processes, covering the upstream processes from material production. The scope reflects the direct area of influence as often only little validated information on the target product and its product life cycle is available at such early stages of development. However, as soon as more information regarding the target product system is available, a (prospective) LCA should be carried out. The aim should be to cover the mutual influence between material, processes, and geometry, which affect the downstream process chain, which is not covered by the introduced calculations. A broader scope also puts the significance of the influence of alloying elements in perspective to the overall impact of a product.

Next to the environmental impact, the recyclability of alloying elements is of major interest, which is not covered by those indicators. The analysis implies that boron is the favorable choice to achieve the required hardenability from a technological, economic, and environmental perspective. The perspective on how well a boron is kept in the anthropogenic system is not considered. Depending on thermodynamics, some elements dissipate from the material, i.e., steel, in the (re) melting process. Considering the established recycling system of steel, this results in a continuous demand for primary material to substitute the losses due to non-functional recycling. Boron reacts with oxygen and nitrogen during remelting, leading to dissipative losses during recycling. These dissipative losses are also claimed to be metals' actual consumption [58]. Steel is considered to have low dissipation ratios because of the established and developed material cycle and its prolonged use phases in the building and construction sector. For alloying elements, this is different, as shown by the metal wheel of Reuter et al. [59].

The introduction of the recyclability of alloys shows that there are further major concepts not covered by environmental analysis, like criticality analysis [60]. It brings together the environmental and economic dimensions as it covers the resource availability and threats from supply disruptions, which can be interesting depending on the underlying question and target group, such as steel producers.

The discussion illustrates conflicting goals that can arise within the alloy design process in the context of sustainability. The best composition exists when optimizing an alloy's hardenability, costs, and environmental impact. Still, the categories do not necessarily correlate. Molybdenum has a strong influence on the costs and a medium influence on the environmental impact. Considering further sustainability variables such as dissipation, longevity, and supply risk, the decision becomes complex, and conflicting goals become clear. To meet most of those variables, the recyclability, the alloy application, and product design should be considered within the development. Boron, for example, has a very low alloy fraction and high losses due to its recycling and would have a very low content in the AHD steel. The expectation is that the metal will likely be lost, which requires primary material. Using the alloy in a durable product could prolong its usage in the anthroposphere.

4.3. *Critical assessment*

Estimating the costs and environmental impact of processes and products is difficult, especially if the required information touches on intellectual property rights or competition-relevant information. This is particularly true for the yield rate of alloying elements during steel production, which differs strongly between companies and even plants. Additionally, when it comes to material sourcing (for example which shares of iron and alloying elements originate from primary production or from recycling), the scrap recipe to pro-duce a steel melt and therefore the initial composition before final alloying adjustment also strongly depends on the steel producer. As a technical discussion on this topic between competitors is forbidden by cartel prevention authorities, no open access data was found and, therefore, was not included in this study. As demonstrated in a previous study, the share of scrap which is used for the steel production has a major influence on the environmental impact [12], which will most likely be more influential than small alloying element additions during final adjustment. It must be noted that the technological question was focused on hardenability only to demonstrate the importance of a comprehensive design approach. Additionally, the assessment of the hardenability was simplified (detailed investigations about the transformation behavior of these steels was published elsewhere [28]) for demonstration purposes. If the proposed framework is applied, or extended to another technical property, reliable models for prediction are necessary to achieve optimum results. Furthermore, all alloying elements have multiple effects on the final steel, which must be considered during optimization. An omission of the molybdenum addition would lead to decreased tempering resistance [6,61,62] of the material or potentially to a change in the scaling behavior [63]. Further expected effects are differences during the steel production, as the slags or the melt itself might be influenced by changes in the chemical composition [53–55].

5. Summary

A comprehensive steel design concept and case study have been presented, considering the impact on the technical property of interest (hardenability), alloying costs, and environmental impacts. It was demonstrated that each alloying element's various environmental impact categories should be assessed for future steel development to minimize the component's impact. The following conclusions can be drawn from this study:

- Evaluating the alloying prices leads to ranking the investigated elements concerning their attributed costs from cheapest to most expensive: boron, manganese, molybdenum, chromium, and nickel.
- For the investigated case, boron is the best choice for increasing the hardenability. The alloying cost for the planet carrier would only increase by 0.01 €, while the change in environmental impact across all categories is the lowest.
- The optimized chemical composition reduces environmental impacts, as the carbon-intensive molybdenum and niobium content can be reduced. The research for comparable data shows that the results align with other studies. It also indicates that the variance of environmental impact for single alloying elements depends on the beneficiation degree and region of production. Still, there is a need for further research to improve the availability of data for all alloying elements.

This paper shows a first attempt to consider the increasing requirements in the field of material design and development. The environmental impact categories - *freshwater ecotoxicity*, *global warming potential*, *human carcinogenic toxicity*, *water consumption*, *cumulative energy demand,* and *total material requirement*, which are found to be the hotspots in the production of alloying concepts were chosen to include the ecological sustainability next to the costs representing the economic dimension. There are a multitude of indicators, especially regarding ecological sustainability. Further aspects should be included, such as the criticality and the behavior of alloying elements in the anthroposphere. Due to limited data, it was rather qualitatively discussed. It shows the potential for a conflict of objectives: boron would be the best choice regarding the technical requirements (hardenability), the costs, and the environmental impact. Regarding its alloy fraction in the overall material flow of steel and its non-functional recyclability, it would be the least favorable choice. This indicates that the end-of-life phase of the material application to close metal loops should be considered, especially when using boron. Otherwise, it will likely be dissipatively lost after a short lifetime. Further, it indicates that the analysis of this study has a narrow scope, which should be widened to further relevant parameters regarding sustainability.

CRediT authorship contribution statement

Alexander Gramlich: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Christoph Helbig:** Writing – review & editing, Methodology. **Moritz Schmidt:** Formal analysis. **Wiebke Hagedorn:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation.

Declaration of competing interest

None.

Data availability

Data will be made available on request.

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Appendix A. Additional information

A.1. Determination of necessary changes to the chemical composition

The following calculations demonstrate how the necessary changes to a steel product's chemical composition can be calculated. From the CCT diagram, it can be concluded that the critical cooling velocity v_c is not high enough to prevent bainite formation. For this specific example, v_c can be calculated as the difference between the temperature after forging (T_F) and the martensite start (M_s) temperature divided by the time required to reach M_s (t_{cool}). This results in a v_c of 1.05 K/s.

$$v_c = \frac{T_F - M_s}{t_{cool}} = \frac{1000^\circ C - 370^\circ C}{600s} = 1.05K\Big/s \tag{6}$$

The produced planet carriers have a real t_{cool} of 2500 s, resulting in a real cooling velocity (v_r) of 0.25 K/s. To achieve the desired microstructure, the critical cooling rate of the material needs to be decreased by

$$\Delta v_{crit} = v_c - v_r = 0.8K/s \tag{7}$$

Δv can then be calculated using Eq. (2). Assuming that only one element is changed to achieve the desired changes leads to the following simplification, as all other elemental contributions and the k0 factor annihilate themselves during subtraction:

$$ln(\Delta v_{crit}) = k_i \bullet \Delta w_i \tag{8}$$

For calculating the required amount of additional alloying elements, Eq. (5) can be rearranged to

$$\Delta w_i = \frac{ln(\Delta v_{crit})}{k_i} \tag{9}$$

If chromium is the element of choice to decrease the vc to the required value, this would result in

$$\Delta w_{Cr} = \frac{ln(\Delta v_{crit})}{k_{Cr}} = \frac{ln(0.8)}{0.50} = 0.45wt\% \tag{10}$$

and therefore, an additional need of 1.01 kg chromium per component (or 1.68 kg of ferrochromium).

A.2. Life cycle assessment

The results show a clear hierarchy of which ferroalloy has the smallest change in environmental impact to achieve the required properties. They depend on the characterization factors for the ferroalloys. Therefore, the variance based on influencing factors such as geographical scope and uncertainties should be considered. The ecoinvent database includes a few datasets, mostly one per alloying element, which is why further studies on the impact of multiple or single alloying elements were considered. One important study is by Nuss and Eckelmann [44]. The article contains a comprehensive overview of 63 metals and their environmental profile.

Table 4
Change in Carbon Footprint per planet carrier – own calculations and comparison to Nuss und Eckelmann [44].

		Cr	Mn	Ni	Mo	B
Calculations	Δkg CO_2 eq	3-8.12	0.5	40.5	9.2	0.01
Nuss and Eckelmann	Δkg CO_2 eq	3.6-4.4	0.4	24.1	0.7	0.01

When widening the scope of literature-based environmental impacts for alloying elements, the possible range of environmental impact becomes clear (Table 5).

Table 5
Overview of Environmental Impact per kg Ferroalloy

Element	GWP [kg CO_2 eq/ kg]	CED [MJ eq/ kg]	Geological Scope	Reference
Chromium	2.4	40.2	Global Average	[44]
Chromium	1.6		Norway	[64]
Chromium	7.2	77	Australia/ Tasmania	[65]
Chromium	5.8		Australia	[64]
Chromium	3.0		Tasmania	[65]
Chromium	2.9		Tasmania	[64]
Chromium	2.4		Finland	[64]
Chromium	5.2		South Africa	[64]
Manganese	1.0	23.7	Global Average	[44]
Manganese	1.8	48	Australia	[65]
Nickel	6.5	111	Global Average	[44]
Nickel	13.9	325	Australia	[65]
Molybdenum	5.7	117	Global Average	[44]
Molybdenum	3.2	29.1	USA	[66]
Molybdenum	14.8	188.6	USA	[66]
Boron	1.6	27.3	Global Average	[44]

The lack of comprehensive data inhibits the display of all influencing factors, such as the diversity of markets. Research has shown significant differences regarding the environmental impacts of alloying elements (Table 5), in particular, the geographical scope, production technology, and the associated energy mix [44] [64,65,67,68]. Evaluating the influence of alloying elements on the environmental impact of steel thus requires a more comprehensive overview of existing studies. Further, the assessment of specific steel types also requires information from the input site about the origin of the alloy input.

Also, there is often no differentiation regarding the quality of alloying elements, meaning the concentrate grade of ferroalloys, which is decisive in steel production, as shown within the research project for the AHD. The ferroalloys needed a certain concentration within the smelting process. Wei et al. [66] also stress the influence of beneficiation degree on the environmental impact. The case study of ferromolybdenum shows that the higher the beneficiation degree, the higher the CF. The impact varies between 14.8 kg CO2 eq (highest beneficiation degree) and 4.7 kg CO2 eq (lowest beneficiation degree) per kg ferromolybdenum with 60 % molybdenum. Such information is only available for a few ferroalloys.

Table 6
Ecoinvent process used to determine the environmental impacts of ferroalloys.

Symbol	Process	Process UUID
B	market for boric acid, anhydrous, powder | boric acid, anhydrous, powder | Cutoff, S	6bd03415-3d54-3590-8071-08ff68f030c8
Cr	market for ferrochromium, high-carbon, 55% Cr | ferrochromium, high-carbon, 55% Cr | Cutoff, S	6a20932a-710d-318b-870d-453de7d275be
Cr	market for ferrochromium, high-carbon, 68% Cr | ferrochromium, high-carbon, 68% Cr | Cutoff, S	0d2ed7a0-2fa4-3ae4-a1a2-7544206888e1
Mn	market for ferromanganese, high-coal, 74.5% Mn | ferromanganese, high-coal, 74.5% Mn | Cutoff, S	2443a8ed-9c6d-31f9-9e64-682719b248bc
Ni	market for ferronickel | ferronickel | Cutoff, S	fcbe54c1-22be-3762-af29-cee7fe53ae84
Ta	market for tantalum powder, capacitor-grade | tantalum powder, capacitor-grade | Cutoff, U - GLO	0ff88397-ba06-3b80-94dc-74608e89f8cd
Mo	market for molybdenum | molybdenum | Cutoff, S	18f0477f-d9d1-3245-8537-661e14c9e222

A.3. Additional optimization

The above-described approach deals with the simplest case: only one element will be changed to reach the desired properties. In reality, more elements are changed during the design process of a new steel alloy. For the present case study, it stands to reason that boron could completely replace molybdenum to save additional costs and CO2 emissions. To determine the boron content required to reduce the molybdenum content to 0.02 wt.-% (trace concentration of molybdenum in iron), the difference in the critical cooling rate for the AHD steel ($v_{c\text{-}AHD}$) and a fictitious, optimized steel ($v_{c\text{-}}$

$_{opt}$) can be set to zero:

$$ln(v_{c-AHD}) - ln(v_{c-opt}) = 0 \tag{11}$$

$$w_{Mo} \bullet c_{Mo-AHD} + w_B \bullet c_{B-AHD} - w_{Mo} \bullet c_{Mo-opt} + w_B \bullet c_{B-opt} = 0 \tag{12}$$

Compared to the initial steel, the concentration of molybdenum is set to 0.02 wt.%, and the boron concentration is inserted as a variable. By converting, the following equation can be obtained.

$$c_{B-opt} = \frac{w_{Mo}}{w_B} \bullet (c_{Mo-AHD} - c_{Mo-opt}) + \bullet c_{B-AHD} = 0.0049 \tag{13}$$

The niobium addition might be omitted to optimize the alloying concept further, as a positive effect on the steel is questionable, as reported in a previous study [9]. As niobium does not notably influence the hardenability (it is not included in Eq. (2)), it doesn't need to be compensated by additional boron. The resulting changes in chemical composition (Mo: -0.22 wt.%, Nb: -0.03 wt.%, B: +0.0024 wt.%) lead to changes in carbon emissions and costs, as displayed in Table 7.

Table 7
Overview of the proposed changes of the chemical composition (Δw_i) and the resulting relative changes per component of alloying costs (Δcosts) and CO_2-equivalent (Δkg CO2-eq).

	Mo	Nb	B	Σ
Δw_i	-0.22 wt.%	-0.03 wt.%	+0.0024 wt.%	-
Δcosts*	-14.35 $	-3.85 $	+0.07 $	-18.13 $
Δ kg CO_2-eq.	-51.78	-18.76	+0.027	-70.51

* The costs for ferro-niobium (66 wt.% Nb) were calculated using the average prices of 2017 to 2020 [50,51].

Table 8
The resulting optimized chemical composition is displayed as AHD-Steel$_{opt}$.

Fe	C	Si	Mn	Cr	Ni	Mo	Al	Nb	B
Balance	0.15	0.50	3.90	0.10*	0.10*	0.02*	0.52	-	0.0049

The second optimization leads to a significant reduction of the CF of the planet carrier. The steel with the lowest environmental impact and economic costs is the optimized chemical composition, using boron to achieve the desired hardenability.

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