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Environmental and economic assessment of hydrogen compression with the metal hydride technology

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Abstract

A critical step in the hydrogen supply chains is the compression phase, which is often associated with high energy consumption and environmental impacts. An environmental and cost analysis of a metal hydride (MH) compressor and competing technologies (an air booster and a commercial hydrogen compressor), is performed for an application to fuel cell driven forklifts. The MH compressor shows limited environmental impacts only when a source of waste heat is available for hydrogen desorption. In these case, impacts would be similar to a generic compressor, but larger than those generated by an air booster. The equivalent economic cost is $6 \in$ per kg of compressed hydrogen for the MH compressor, which is much higher than for the air booster, but lower than for a generic hydrogen compressor. Technical aspects to be improved for large-scale applications of MH compressors are identified.

Keywords: Metal hydride; hydrogen compression; Life Cycle Assessment; economic analysis

1. Introduction

According to the International Energy Agency, it will be challenging to reduce fossil fuels consumption in the energy and heat sectors, as well as in the transport and industry sectors; in fact, these are the sectors that today have the highest energy demand [1]. To address these requests, one solution is to positively promote electricity generation from renewables to substitute fossil fuels consumption, while increasing the efficiency of energy conversion. The European Union, on its path towards a reduction of greenhouse gas emissions and an increase in renewable energy, has set the ambitious goal of reaching at least a share of 32% of energy production from renewable sources by 2030 [2]. In this scenario of change, hydrogen is thought of as an important energy carrier, that can be used for the storage of renewable energies [3-6] and have great potential in stationary, portable and transport applications [7,8]. Europe has recognized as significant and stimulating elements in the deployment of a hydrogen economy: (i) the reduction of climate change effect, (ii) the enhancement of energy security and (iii) the promotion of renewable energy exploitation. However, the implementation of a hydrogen economy still presents various challenges from the point of view of technological maturity, infrastructures availability, and effective regulations and standards [9,10].

In the transportation sector, there is a great interest for the benefits derived from the application of Proton Exchange Membrane fuel cells (PEM FC). It has been found that such environmental benefits, in terms of Greenhouse gas (GHG) reduction, can be substantial with the use of hydrogen produced from renewable energy sources [11–14]. An interesting and promising application

market, for fuel cell technology, is that of vehicles for handling units / forklifts. Some reports, which have conducted market analyses on this topic, confirmed that under certain conditions (e.g. energy efficiency, fleet size, etc.), the fuel cell forklifts show advantages, both in economic terms and in the possible reduction of energy consumption and GHG emissions [15,16].

From the technological viewpoint, the use of hydrogen as an energy carrier is slowed down by some issues: one of the main ones is undoubtedly that hydrogen production needs energy to be produced, being only an energy carrier and not an energy source [17]. On the other hand, to enable and spread this technology, it is also necessary to study and improve other aspects, such as hydrogen storage, transportation and distribution. A not negligible point that deserves to be carefully examined is the gas compression. In fact, hydrogen has the lowest volumetric energy density among the commonly used fuels [18]. To overcome this aspect and increase the volumetric energy density, one of the most used approaches is gas compression. The compression of hydrogen at high pressures is required for specific applications; as an example, for the transport sector, hydrogen needs to be pressurized above 700 bar to enable refuelling of high-pressure storage tanks of a car [19]. The need to increase gas pressure makes it possible to optimize storage and makes the hydrogen transportation and use viable [20]. It should be noted that, in counting the benefits deriving from the use of hydrogen as an energy vector, the entire supply chain must be considered: the primary energy used for its production, compression, storage, transport and final use [21]. The compression phase has to be considered with care, because it is an operation that has a high energy demand [21,22]. In fact, if the hydrogen compression is not managed carefully, it can cause an energy loss of up to 20% of the hydrogen energy content [21].

Currently, there are several different technologies for hydrogen compression, each with specific advantages and drawbacks. For example, mechanical compression is the most widespread approach for compressors used nowadays, which use mechanical energy to compress gases [20]. The so-called reciprocating compressors, which represent a mature technology, adaptable to a wide range of gas flow rates, belong to this family; they consist of several moving parts, but this feature increase both the cost of manufacturing and the difficulty in carrying out effective maintenance [23]. At the same time, the presence of moving parts, like the piston, leads to an increase in the heat produced and makes more difficult to manage thermal transfers [24].

An interesting alternative, that does not require moving parts, is represented by the use of metal hydride to compress hydrogen, known as thermally-driven compression [20]. The compression with metal hydride is based on the reversible reaction between hydrogen and a solid phase (an elemental metal, alloy or intermetallic compound). Hydrogen absorption is an exothermic process, implying the release of heat, while desorption is endothermic, so that hydrogen is released only upon the supply of heat. Fig. 1a shows equilibrium absorption and desorption curves of H₂ by means of a solid phase. For a fixed temperature, because of the hysteresis effect, the hydrogen absorption (A) is obtained at a higher pressure with respect to the desorption (D). The solid phase (M) can absorb H₂ at low temperatures (T₀) and pressures (P_A), forming the hydride (MH). Then, by heating MH at higher temperatures (T₁), H₂ is released at a higher pressure (P_D). If reactors with different solid phases are connected in series, the final pressure can be further increased, as shown in Fig. 1b. By cycling between T₀ and T₁, hydrogen can follow successive compression stages, as shown in steps 1, 2, 3, 4 in Fig. 1b.





According to Lototskyy et al. [25], this technology has several advantages, such as the absence of moving parts, so it does not require frequent maintenance, it is compact and safe and, for the operation phase, offers the possibility of using industrial waste heat.

The use of metal hydride compressors in forklifts refueling stations is particularly suited, because the pressure needed for the storage of hydrogen in forklifts is about 200 bar, a value that can be easily obtained with commercial metal hydride compressors [26,27]. Moreover, it is likely that in the place where the refueling station is located (a factory), excess heat to operate the compressors is available from other processes. In fact, one of the main advantages of this technology is that, for its operation, a metal hydride compressor only needs a source of heat (a hot fluid such as steam between 130 -150 °C) and water for cooling (temperature below 25 °C) [27,28].

In the literature, apart some techno-economic analyses of hydrogen refuelling stations [21,22,,29] which have also taken into consideration the compression phase, there is a lack of specific studies focused on the environmental and economic performances of various compression technologies. In this work, the environmental performance of a metal hydride compressor has been assessed by means of the Life Cycle Assessment (LCA) methodology. The goal of the study is to quantify advantages and disadvantages of a MH compressor, with respect to more mature competing technologies. The expected result is the identification of the main environmental hotspots, in order to obtain indications on how to make this type of technology more sustainable and competitive. This study has been inserted in a wider context by comparing the MH compressor with two different commercially available systems for hydrogen compression, to provide a better understanding of the environmental and economic performances of the MH compressor and identify which technology is the most suitable for specific uses. More in details, this analysis compares the technology of a MH compressor, a generic H₂ compressor and an air booster.

This work is structured as follows: section 2 reports the environmental analysis, carried out by means of the LCA methodology and it is organised in 4 sub-sections, representing the four phases of an LCA (goal and scope definition, life cycle inventory, life cycle impact assessment, and interpretation); section 3 shows the method and results of the economic analysis; finally, section 4 summarizes the main results obtained from this study.

2. Life Cycle Assessment

LCA is an environmental management tool for quantifying, interpreting and evaluating the environmental impacts potentially caused by a product or a process along its entire life cycle. This methodology quantifies the amount of resources, raw materials, energy used and the emissions and wastes over the complete life cycle of goods or services [30]. According to ISO 14040 and 14044 standards requirements, four stages are needed to conduct an LCA: goal and scope

definition, life cycle inventory (LCI), life cycle impact assessment (LCIA) and results interpretation [31,32].

This work applies the LCA methodology to investigate the environmental impacts associated with the hydrogen compression phase in a refuelling station for fuel cell forklifts. The attention was focused only on the compression phase and three different systems were analyzed and compared: a metal hydride compressor, a generic H_2 compressor and a system that uses an air booster to increase the hydrogen pressure.

The entire work was conducted with software SimaPro 9.2 and using the Ecoinvent v.3.7.1 database.

2.1. Goal and scope definition

Goal and scope definition is the first step of the analysis, and it defines the object of the study, the system boundaries and the functional unit for all flows. The main goals of the work can be summarized as follow:

- Quantify the environmental burdens related to the production of a MH compressor and identify the main hotspots related to it.
- Quantify the environmental impacts associated with a MH compressor use phase, comparing different scenarios: the use of waste heat and cooling from another system, use of electricity generated by a photovoltaic system, direct use of natural gas to heat the system and use of energy from the electrical national grid.
- Compare the system under analysis with systems providing the same services, i.e. generic H₂ compressor and air booster. This comparison takes into account also the use phase of the systems.

The same compression rate and final pressure were considered for all considered compressors.

The functional unit identified for this study is the compression of 1.79 kg of H_2 , at 200 bar, in 7 hours, therefore the dimensions of the integrated system have been modelled to achieve this goal. The choice of the amount of hydrogen to be compressed was based on the daily operation of a forklift [28,33]. For the sake of clarity, it should be noted that the compressed gas is not immediately directed to the forklift tank, but it is stored in a buffer tank. In this way, it is not necessary to use compressors with high hourly flow rates of compressed gas. This configuration is preferred because, in economic terms, it is cheaper to have a small compressor that works almost all day than a large compressor working for short times [21].

The environmental impact assessment was carried out by selecting six impact categories deemed most relevant among those recommended by the European Commission [34]. The considered impact categories, corresponding units and the related methods used to calculate them are shown in Table 1.

Impact category	Unit	LCIA method used
Climate change	kg CO2 eq	Baseline model of 100 years of the IPCC [35]
Particulate matter	Disease incidences	PM method recommended by UNEP [36]
Photochemical ozone formation	kg NMVOC eq	LOTOS-EUROS [37]
Acidification	mol H⁺ eq	Accumulated Exceedance [38,39]
Resource use, energy carriers	MJ	ADP for energy carriers, based on [40] as implemented in CML, v. 4.8 (2016).
Resource use, minerals and metals	kg Sb eq	ADP for mineral and metal resources, based on [40] as implemented in CML, v. 4.8 (2016).

Table 1 List of impact categories, corresponding metrics and methods used.

2.2. Life cycle inventory

The life cycle inventory, the second phase of a LCA study, has the purpose of identifying and quantifying the elementary flows between the foreground system and the environment in the life cycle of the process or product under study. The complete list of raw materials, resources, energy, outputs, and emission related to the considered functional unit was compiled and a model was built in SimaPro. The data that constitute the inventory of this study derive both from direct measurements on the system (primary data) and from the literature.

Details of the inventory of the various components taken in consideration for the MH compressor, the air booster and a generic H_2 compressor are reported below.

2.2.1. Metal hydride compressor

The data to model the metal hydride compressor were estimated by considering, as starting information, a real MH compressor, studied and developed by the University of Turin and Tecnodelta s.r.l. (Fig. 2).



Fig. 2 a) Picture of the metal hydride compressor prototype used for this study; b) simplified diagram with details of the two reactors.

The prototype, used as reference, is made up of two reactors placed in series and connected by a valve system. Two different metal alloys in the form of powder are placed inside the reactors; when these alloys react with hydrogen, they form the metal hydrides enabling the consequent operation of the compressor.

The materials used for the reversible sorption of hydrogen are $La_{0.9}Ce_{0.1}Ni_5$ and $Ti_{0.95}Zr_{0.05}Mn_{1.55}V_{0.45}Fe_{0.09}$ commercial alloys in the form of powders. Each of these reactors consists of an internal tube surrounded by an external jacket, that enables the control of the temperature [41]. During hydrogen absorption or desorption, a fluid for the heating and cooling

steps is flowing between the internal pipe and the external jacket, both of them in stainless steel. The outer jacket is thermally insulated from the environment by a layer of glass fibre.

The system is assembled so that the gas, coming from the hydrogen source, reaches the first reactor and, after the absorption/desorption stages, it flows into the second reactor and, finally, it reaches a tank, where it is stored. To clarify the operation of the MH compressor, a description of a single compression cycle is given, with reference to Fig. 1b: the H₂ gas at low pressure (\approx 30 bar, P_{A1}) flows in the first reactor, that is kept at room temperature (T₀), and it is absorbed by the first alloy. Then the reactor is heated (130 – 150 °C, T₁) and the hydrogen is released at a pressure (P_{D1}) greater than 30 bar, flowing into the second reactor. In this phase, the second reactor is kept at room temperature (T₀) and the second alloy absorbs (P_{A2}) the incoming H₂. As a last step, the second reactor is heated (T₁) and consequently the H₂ is released at 200 bar (P_{D2}) to a storage tank. The developed system allows the compression of 0.052 kg of hydrogen at 200 bar with 7 absorption/desorption cycles for each reactor. Since the duration of 1 cycle is approximately 1 hour, a total of 7 hours is required to compress the desired amount of hydrogen.

Data measured with the previously described prototype were used as input for the modelling, scaling up to the compression, at 200 bar, of a greater quantity of H₂ (i.e. 1.79 kg) in 7 hours. The amount of each alloy was estimated by knowing the respective reversible hydrogen storage capacities, and the hydrogen flow needed to obtain 1.79 kg of compressed gas in 7 hours. The first step of absorption/desorption takes place in the first reactor, using 21.31 kg of La_{0.9}Ce_{0.1}Ni₅ alloy (reversible hydrogen storage capacity 1.2 wt%). The second step is carried out into the second reactor, containing an alloy with composition Ti_{0.95}Zr_{0.05}Mn_{1.55}V_{0.45}Fe_{0.09} (15.98 kg, reversible hydrogen storage capacity 1.6 wt%). The amount of single elements in each alloy is reported in Table 2.

Alloy	Element	Amount (kg)	Input (inventory)
La. Co. Ni.	La	5.75	
21 31 kg	Ce	0.75	LaNi ₅ (electrode material)
21.51 kg	Ni	14.81	
	Ti	4.48	Titanium (primary)
Ti7rMnVFo	Zr	0.48	Zirconium*
15.98 kg	Mn	8.31	Manganese
	V	2.24	Titanium (primary)
	Fe	0.48	Cast iron

 Table 2 Elemental composition and inventory inputs of the two commercial alloys. *The process to obtain Zr was reconstructed with data from literature [29]

Given the lack of specific data within the Ecoinvent database, for the $La_{0.9}Ce_{0.1}Ni_5$ alloy, the process used to produce $LaNi_5$ (electrode material for batteries) has been considered, neglecting the contribution given by the small amount of Cerium. The Ecoinvent database does not contain any data for the elemental Zirconium, so the process for its production was reconstructed starting from the corresponding oxide, according to Nuss and Eckelman [42]. Also for the Vanadium there are no data in the literature or commercial dataset with sufficient quality to model its contribution. It was therefore chosen to use the titanium process as a proxy. The quantity of titanium, used for the modelling, is equal to the value of requested vanadium multiplied by a numerical factor of 1.1, as suggested by Nuss and Eckelman [42].

The size of the steel tubes was defined using commercial pipes that allow to contain the quantity of alloys (with 30% of free internal volume) and to withstand the temperatures and pressures reached during the desorption reaction (150 °C and 200 bar). The modelled system consists of four

stainless steel 316 tubes (length: 166 cm, internal diameter: 3.3 cm, external diameter: 4.2 cm), each of which is enclosed in a larger outer jacket, also in stainless steel. The section between the two tubes contains the thermal fluid, therefore the external tube is surrounded by a glass fibre for thermal insulation.

The inventory of the MH compressor is reported in Table 3.

Input	Amount
Stainless steel (kg)	330
Metal working (kg)	330
La _{0.9} Ce _{0.1} Ni ₅ (kg)	21.31
Ti _{0.95} Zr _{0.05} Mn _{1.55} V _{0.45} Fe _{0.09} (kg)	15.98
Glass fibre (kg)	34.42
Pump 40W (unit)	12

Table 3 Inventory for the compressor system with metal hydrides.

The amount of stainless steel reported in Table 3 refers to the reactors, pipes, connections, valves and structural frame that make up the entire system. This quantity of material is quite substantial compared to other MH compressor systems reported in the literature, where a ratio of alloys over stainless steel is determined around wt. 30% [27,43-45]. Since this ratio for the developed prototype system is around wt. 12%, it can lead to an overestimation of the environmental impacts generated by the MH compression technology. For this reason, in addition to evaluating the environmental impact generated by the system modelled with the data shown in Table 3, the study was expanded by modeling the same compressor with a lower steel input, in order to achieve an alloy:steel ratio of wt. 30% and wt. 40%. In fact, these values can better represents a large scale metal hydride compressor, with optimized design.

The pumps allow the circulation of the thermal fluids responsible for heating and cooling the system. The fluid for heat management was not considered in modelling the inventory, because there are several possibilities (water, water-glycol mixture, steam, electrical resistance, air, etc.) and all of them have a very limited environmental burden compared to the total impact of the system.

At the moment, there are few studies regarding the life span and performance over time of the technologies used in the MH compressors. For example, Tarasov et al. [46] reported quite encouraging information about Lanthanum-Nickel alloys; in fact, they observed that up to 10000 cycles, the average productivity decrease by only 5 – 10% and that the degradation of these solid phases is mainly due to the number of absorption/desorption cycles. So with a good approximation, we assumed the possibility of cycling the alloys for a number of 10000 times. Assuming a daily compression of 1.79 kg of hydrogen with 7 cycles, it means that the alloys will have to be replaced, on average, every 5.5 years (taking 253 working days per year). It should be noted that the possibility of restoring the original capacity of the alloys can be obtained thanks to specific thermal treatments [25]. In this way, the solid phases used for the absorption and desorption of hydrogen could be used indefinitely. Given the lack of more precise information to model these treatments on an industrial scale, we considered the full replacement of alloys, even at the cost of overestimating environmental impacts.

Since the steel structure, which constitutes the reactors and the gas lines, is subjected to repeated work cycles, it was assumed that it must be replaced every 10 years. Also, the glass fibre and the pump have been considered to be replaced after 10 years of use.

The amount of energy used during the compression of 1.79 kg of H₂, at 200 bar, to operate the compressor in the absence of a waste heat source, was determined bearing in mind the mechanism of gas desorption from the solid phase (endothermic reaction). The estimation was obtained considering the energy contributions to provide the heat necessary to reach and maintain a suitable temperature allowing the desorption of hydrogen in the outer jacket, the steel pipes, and the alloys. Moreover, the heat consumed during the desorption of the H_2 from the alloy itself and the energy consumed by the cooling system were also considered. The estimated energy consumption related to the functional unit turned out to be equal to 50 kWh. The system was modelled using both electricity coming exclusively from solar energy (Electricity, low voltage {IT}) electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted), energy taken from the grid (Electricity, low voltage {IT} | market for) and heat produced by natural gas (Heat, central or small-scale, natural gas {Europe without Switzerland}] market for heat, central or small-scale, natural gas | Alloc Rec, U). It should be noted that the heat necessary for the operation of the MH compressor could be also obtained from a solar thermal system. In this case, impacts generated could be lower than other energy sources; however, since this scenario would have required additional modelling and assumptions, as commercial datasets are available only for low temperature household systems, it was preferred to neglect this possibility in this analysis.

2.2.2. Air booster

The hydrogen compression at high pressure can be realized also by means of a booster, a device using a low pressure air flow to increase the pressure of the desired gas. In this case, a commercial booster suitable for the oil free compression of gases and air was considered. The use of an air booster to raise the pressure of a gas is particularly suitable in cases where high hourly flow rates are not required and only for not continuous uses of the booster (there is no cooling system). These two conditions are fully fitting for the application reported in this study.

The main constituting materials and relative amounts are reported in Table 4; some materials, due to their very low relative weight, have been neglected. In the modelling, a 10-year lifespan for the air booster was assumed.

Material	Amount (kg)
Stainless steel	19.5
Metal working (kg)	19.5
Acrylonitrile-butadiene-styrene copolymer	0.20
Polypropylene	0.15

 Table 4 Inventory for the commercial booster.

To operate, the booster requires only a flow of air, in a range pressure of 4-8 bar, easily obtained from an air compressor. In the Ecoinvent database, there is a process that allows to directly obtain the environmental impacts related to the production of a specific amount of compressed air. In this case, 1.2 m³ of air are required to compress 1.79 kg of H₂ up to 200 bar, using an air driving pressure of 6 bar. The electricity consumption associated with the production of 1.2 m³ of compressed air is 0.238 kWh; this energy contribution was modelled using, in one case, electricity from the Italian grid and, in an alternative case, electricity produced from a photovoltaic system. It should be noted that the compression phase carried out with the booster is not continuous, but requires long rest times as the system is not cooled and therefore approximately 7 hours are required to compress 1.79 kg of H₂ at 200 bar (the chosen functional unit). For this reason, the overall energy consumption of this system is very limited.

2.2.4. Hydrogen compressor

As reported in the literature [20], there are various technologies marketed for the compression of hydrogen: mechanical compressors, cryogenic compressors, electrochemical compressors, and adsorption compressors. However, given the lack of primary and/or secondary data to model the compression of hydrogen using one of the previously mention technologies, it was decided to use the environmental impacts present in the Ecoinvent database related to an air compressor (screwtype 4 kW). This assumption tends, with high probability, to underestimate the impacts associated with the compressor itself. In fact, due to the properties of the substance to be compressed, a compressor for hydrogen undoubtedly requires more efficient materials and technologies than an equivalent for air. The contribution of the compressor has been scaled by assuming that it has a life span of only 10 years, which was chosen to compensate for the difference in technology of the screw type compressor compared to a generic H_2 compressor. The energy consumption for the hydrogen compression was obtained from the literature [47], leading to a value of 5.9 kWh for the functional unit. Also in this case, the system was modelled using both electricity from the grid and electricity from a photovoltaic system. The production of energy, in both cases, always refers to the Italian context. The energy consumption in this case is higher than using the air booster, as a generic hydrogen compressor requires a precise temperature management system. In addition, a generic compressor has an efficiency far greater than that of the two previous systems; it should be noted that the reported energy consumption value has been scaled with respect to the quantity of compressed H₂ and it is therefore independent of the time required to complete the compression.

2.3. LCIA results

The large number of elementary flows of resources and emissions associated to the inputs and outputs of the inventory, have been transformed, with the life cycle impact assessment methods, into a handful of environmental impact categories, as reported in Table 1. Fig. 3 shows the results of all impact categories analysed to produce of one unit of MH compressor. The results were reported as a percentage of the total impacts for each category; Table A.1 in Appendix A reports the corresponding numerical results.



Fig. 3 LCIA results, express as a percentage of the total, to produce of the MH compressor.

From results shown in Fig. 3, related to the production of a MH compressor, it can be observed that the greatest impacts are attributable to the amount of stainless steel used and to its working. In fact, for all considered categories, the environmental impacts generated by the production and processing of steel are around, or slightly higher, than 50% of the total impact (in detail: 62% for climate change, 61% for particulate matter, 56% for photochemical ozone formation, 49% for acidification, 61% for resource use, energy carriers and 44% for resource use, minerals and metals). The metal alloys, on which the operation of the compressor is based, have lower impacts, despite requiring elements in the oxidation state 0; in fact, elements in this oxidation state generally involve high environmental costs for their production. In detail, the impacts of $La_{0.9}Ce_{0.1}Ni_5$ alloy, relating to the acidification category, are due to the nickel mining processes, while for all the other categories considered, they are caused by the extraction and processing of the element belonging to the rare earth groups (La); the extraction of rare earth elements and the manufacturing processes involve the use of considerable amount of hydrochloric acid, sodium hydroxide and energy, that are the main responsible for the impact among analyzed categories. The results related to the second alloy, Ti_{0.95}Zr_{0.05}Mn_{1.55}V_{0.45}Fe_{0.09}, are mainly due to the amount of titanium used, for all impact categories. The impacts associated with titanium are caused by the high energy consumption required for its industrial extraction and purification. The glass fiber, used as thermal insulation, shows the lowest impacts for each category. The high impact associated with the pump, for the category resource use, minerals and metals, is due to the amount of copper present inside this device; it must be said that such impact can be significantly lowered, taking into account the possibility of recycling this element.

Figure 4 shows the results for the Climate change category obtained by modelling the MH compressor reducing the amount of stainless steel for its production. In detail, the figure shows the impact for the previously shown case (original data), for the MH compressor modelled with a ratio alloys:steel equal to wt. 30% (MH:SS 30%) and for the MH compressor modelled with a ratio alloys:steel equal to wt. 40% (MH:SS 40%).



Fig. 4 LCIA results for the Climate change category for the production of the MH compressor modelled with different ratio alloys:steel (MH:SS)..

Results reported in Fig. 4 shows how a reduction in the amount of stainless steel, used to build the system, allows to reduce the environmental impact. Indeed for the cases modelled with a ratio MH:SS of wt. 30% and wt. 40%, the overall emission of carbon dioxide in the atmosphere can be decrease respectively of 38% and 44%. By modelling the MH compressor in this way, it became clear that the environmental contribution of the two alloys, specifically of the La_{0.9}Cr_{0.1}Ni₅ is absolutely unneglectable, but rather the main cause of the impact of the system.

An equivalent contribution analysis was not carried out neither for the air booster nor for the generic H_2 compressor. In fact, it was considered that the results would have been scarcely informative, as the air booster was made almost entirely of steel and the generic compressor was instead modelled using the Ecoinvent dataset relating to an air compressor.

The environmental impacts generated by the compression of 1.79 kg of H₂, at 200 bar, were evaluated by comparing several systems:

- metal hydride compressor that uses a waste heat source (MH comp)
- metal hydride compressor that uses heat from natural gas (MH comp + heat NG)
- metal hydride compressor that uses electricity from the grid (MH comp + grid el)
- metal hydride compressor that uses electricity from a photovoltaic system (MH comp + PV el)
- air booster that uses electricity from the grid (air booster + grid el)
- air booster that uses electricity from a photovoltaic system (air booster + PV el)
- hydrogen compressor that uses energy from the grid (H₂ comp + grid el)
- hydrogen compressor that uses electricity from a photovoltaic system (H₂ comp + PV el)

Figure 5 shows the results, for each impact category, obtained by comparing the various compression systems; the numerical values of the calculated impacts are reported in Table A.2 in Appendix A. The impacts, related to the hydrogen compression in accordance with the functional unit, were reported by dividing the total into two contributions: impact due to the system (i.e. impact due to the production of the compressor, normalized for its life span) and impact generated by energy consumption to compress the gas.



Fig. 5 Comparison of the environmental impacts associated with the compression of 1.79 kg of H₂ at 200 bar using different systems. Impact categories: a) climate change, b) particulate matter, c) photochemical ozone formation, d) acidification, e) resource use, minerals and metals, f) resource use, energy carriers.

Fig. 5a shows how, for the climate change category, the main burdens are associated with the MH compressor. that needs an external energy source to operate; the greatest impacts are generated by using electricity from the national grid, followed by heat from natural gas and electricity from a photovoltaic system. The high energy consumption associated with the MH compressor, when a source of waste heat cannot be used, is the main cause of the high greenhouse gas emissions. It is worth noting that the use of energy from the national grid involves the greatest impacts ($\approx 23 \text{ kg}$ CO₂ eq), while the use of heat obtained from the combustion of natural gas allows to reduce considerably the impact ($\approx 15 \text{ kg}$ CO₂ eq). An even better result is obtained by using electricity produced by a photovoltaic system ($\approx 5 \text{ kg}$ CO₂ eq). As expected, the use of the MH compressor, with waste heat recovered from an external source, allows to contain the environmental impacts related to the H₂ compression. The emission of CO₂ eq. is slightly lower than that generated by the compression using a generic H₂ compressor that uses energy from the national grid, respectively 1.77 and 2.82 kg CO₂ eq. Based on greenhouse gas emissions, the best way to compress H₂ is through a booster that uses compressed air; the impacts are minimal if compression is done using electrical energy produced from a photovoltaic system ($\approx 0.07 \text{ kg}$ CO₂ eq).

The results related to the category particulate matter, expressed as disease incidence, are reported in Fig. 5b. The relative trend for different technologies is guite similar to that obtained for the climate change: the greatest impact is observed using the MH compressor which uses electricity from the national mix and the lowest is always obtained from compression with the booster and air compressor system. However, some differences can be noted. In fact, the impact generated by the compression with the MH compressor alone (without the use of energy) reaches higher values than the generic H₂ compressor. About 61% of the impact generated by the MH compressor is due to the stainless steel (materials and processing) used to build the system (Fig. 3). In particular, a large part of the particulate emission derives from the energy spent during the extraction phases of minerals used for the production of stainless steel, i.e. ferronickel and ferrochromium. The production of electricity through a photovoltaic system causes a greater emission of particulate matter compared to an equivalent amount of heat produced by the combustion of natural gas. This major impact is attributable to the production phase of silicon for the photovoltaic panels. It can be observed that the system that uses a generic H_2 compressor shows greater sharing of the impacts, both by the physical system and by the energy used, compared to the impacts on climate change; in fact, the impact on the climate change category is strongly caused by energy consumption. On the contrary, the use of metals (steel, aluminum and copper) in the generic compressor involves an emission of atmospheric particulate that has a greater relevance in this category.

Fig. 5c shows the impact related with the photochemical ozone formation. The release of tropospheric ozone precursors (measured as NMVOC eq.) into the atmosphere is particularly noticeable for hydrogen compression that uses electricity produced with the Italian national mix. This impact is largely due to the percentage of electricity that derives from the use of coal as an energy source. It is worth noting that there is only a slight difference in terms of NMVOC eq. emissions when using heat produced from natural gas or electricity obtained from solar energy. Again, the system consisting of booster with air compressor proves to be the best from an environmental point of view. The impacts associated with compression using the hydride system alone are limited and are slightly lower than using a generic compressor powered by electricity from the Italian grid.

The results related to the acidification impact category are shown in Fig. 5d. The comparison among the impacts related to the acidification category proposes a similar trend to those previously observed: the compression of hydrogen with the metal hydride system, that uses electricity, causes once again the greatest impacts, whereas the best solution is represented by the booster with air

compressor system. The high impact associated with the use of energy produced using the Italian energy mix derives from the combustion of coal. Although this contribution corresponds to only 14% of the total energy production (year 2016), it is the cause of 50% of the total impact. In fact, during the coal combustion, nitrogen and sulfur oxides are released into the atmosphere which, when deposited, can cause a decrease in the pH of soils and fresh water. It should be noted that coal is subjected to treatments for the removal /abatement of sulfur species and nitrogen oxides, but these treatments do not allow a complete removal of these chemical species. The use of energy produced by a photovoltaic system shows higher impacts compared to the production of heat, deriving from the combustion of natural gas; these greatest impacts find their origin in the production phases of crystalline silicon and in the other components used in solar panels. As shown in Fig. 3, the impact generated by the MH compressor is split between the inputs of the stainless steel and the nickel, present in the first alloy. The emission of acidifying substances of the MH compressor (0.014 mol H⁺ eq) is almost the same than that generated by compression with the generic H₂ compressor, which uses energy from the national grid.

Fig. 5e shows the comparison of the depletion of minerals and metals caused by the different processes of H_2 compression. With respect to the categories previously considered, a change in the relative impacts is evident: in this case, the system that uses the MH compressor, powered by solar energy, causes the greatest impacts. The burdens associated with the use of photovoltaic panels are generated by the use of metals such as steel, copper and silver in the panel production chain. It is interesting to underline that the use of alloys, i.e. transition metals and rare earths, does not generate such a marked impact. Only around 20% of the MH compressor impact related to resource use is caused by the alloys, whereas the remaining fraction is almost entirely due to stainless steel. The impact generated by the MH compressor is very similar to that obtained for a generic H_2 compressor. It should be noted that the latter was modelled by assuming that the generic H_2 compressor is similar to a common air compressor; therefore, the impact for this category may likely be slightly underestimated.

Fig. 5f shows the primary energy consumption (in MJ of fossil fuels) consumed using compared systems for the H_2 compression. This impact shows a similar trend as for the impact related to climate change. The best system is always represented by the air booster and the worst by the MH compressor powered with energy from the grid. This result is not surprising, because both impacts are strongly related to energy consumption. The use of electricity from a photovoltaic system makes it possible to greatly reduce the consumption of fossil resources, however the resources consumption remains higher than that of the other systems for compressing H_2 . The impact generated by the MH compressor (without energy consumption) is half the impact generated by the use of a generic H_2 compressor that operates with electricity from the national mix (19 MJ and 40 MJ respectively).

Overall, results reported in Fig. 5 made it possible to identify that the best solution to compress hydrogen, from an environmental perspective, is to use a system based on a booster coupled to an air compressor. It should be noted that this conclusion is valid for the specific functional unit analyzed here: the compression of 1.79 kg of H₂ at 200 bars in 7 hours. The metal hydride compressor, modelled on the basis of available data, generates significant environmental impacts, especially when it is unable to use a source of waste heat. In fact, the energy to be supplied as heat to carry out the hydrogen desorption is quite high. The environmental impacts remain much higher than all alternatives, even by using renewable sources (i.e. electricity produced by a photovoltaic system) or by producing heat by direct combustion of natural gas. For certain categories analyzed (i.e. climate change, photochemical ozone formation, resource use, energy carriers and resource use, minerals and metals) impacts generated by compression with a metal hydride system, that takes advantage of a waste heat source, are slightly lower than those produced during compression with a generic H_2 compressor. Instead for the category particulate matter a marked difference remains between these two systems.

Optimized MH compressors requiring a lower amount of structural materials for construction, as reported for the cases analyzed in Fig. 4, would of course generate lower environmental impacts as regards the contribution of the physical system construction, however the impacts from the manufacturing would still be higher than the other systems for all impact categories but resources depletion minerals, for which, in nay case, the MH would be in between the booster and the generic compressor.

3 Economic analysis

The comparison between the three H_2 compression systems has been extended to include a cost analysis. The costs of the alloys that make up the MH compressor have been obtained by the companies that sell these materials on the market; the cost of the other materials making up the MH compressor were obtained from an online market research. The cost of the air booster refers to a specific device directly purchased. The prices of the air compressor and the generic H_2 compressor correspond to average values obtained from various quotations obtained via web search.

Fig. 6 shows the cost distribution among the main components of the three considered systems. The detailed costs for the three system are reported in Table A.3 in Appendix A.



Fig. 6 Capital cost of analysed hydrogen compression systems.

The greatest investment is for the generic H_2 compressor, followed by the MH compressor and finally by the booster with air compressor system. The MH compressor has a capex equal to around a quarter of the generic H_2 compressor and only slightly higher than the booster coupled to an air compressor. The main costs for the MH compressor are attributable to the alloys, in particular to the La_{0.9}Ce_{0.1}Ni₅ alloy.

Since it has been assumed that the compression systems can be powered by energy from different sources, Table 5 shows the prices of electricity corresponding to the Italian mix and electricity produced with a photovoltaic system.

	Electricity Italian energy mix	0.15	€/kWh	[48]
Energy	Solar photovoltaic	0.05	€/kWh	[49]

 Table 5 Price of the energy used to model the systems.

Fig. 7 shows the cost of the hydrogen compression, per functional unit, distributed among the main components of the three systems modelled. The cost of energy was also considered among all contributions. It was assumed that the MH compressor operates using recovered heat, while the air compressor for the booster and the hydrogen compressor use electricity from the Italian national mix. Table A.4 in Appendix A reports the corresponding numerical cost.



Fig. 7 Cost for the compression of 1.79 kg of H₂, at 200 bar, with the three systems analyzed. Because waste heat was considered to be supplied to the MH compressor, no energy costs were considered in the case. The use of energy from the Italian national mix was assumed to power the system with booster and the generic compressor for H₂.

The inclusion of the cost of the electricity for the air booster and H₂ compressor does not change significantly the results. The compression of 1.79 kg of hydrogen, at 200 bar, costs 10.7 \in using the MH compressor, 2 \in with the air booster and 29 \in with a generic H₂ compressor. If energy produced by a photovoltaic system were used, the cost related to energy consumption would be even more limited, as indicated in Table 5. The higher cost for the hydrogen compression originates from the investment for the purchase of the H₂ compressor, whereas considering the MH compressor, the alloy La_{0.9}Ce_{0.1}Ni₅ causes the highest costs. As regards the compression carried out with the air booster system, almost all of the cost derives from the purchase of it.

From an economic point of view, the most economical way to compress hydrogen, under the specific conditions defined in this work, is the booster system coupled with an air compressor.

4. Conclusions

The main novelty brought by this study is an environmental and economic assessment of hydrogen compression technologies; in fact, currently in the literature there is no evaluation of the environmental impacts generated either by MH compressors or by other technologies for hydrogen compression. For the function (compression of hydrogen for a forklift) and the functional unit (1.79 kg H_2 at 200 bars in 7 hours) used in this study, it was found that the best solution to compress hydrogen, both from an economic and environmental perspective, is to use a system based on a booster coupled to an air compressor.

The metal hydride compressor shows limited environmental impacts, only when it is possible to use a source of waste heat (e.g low grade steam) for the hydrogen desorption phases. In this case, the LCIA results for the compression of 1 kg of hydrogen are: 0.98 kg CO₂ eq (climate change); 3.7*10⁻³ kg NMVOC eq (photochemical ozone formation); 7.3*10⁻³ kg disease inc. (particulate matter); 7.9*10⁻³ mol H⁺ eq (acidification); 12.05 MJ (resource use, energy carriers); 3.9*10⁻⁵ MJ (resource use, minerals and metals). The equivalent economic cost is 6 € per kg of compressed

hydrogen. These results although lower, or similar, compared to those obtained using a generic H_2 compressor, are larger than the environmental impacts generated by using an air booster. The use of the MH compressor, which requires a dedicated energy source (like heat from natural gas, electricity from the national grid or electricity from a photovoltaic system), has a greater impact when compared to all the other solutions analysed.

An interesting result is the significant environmental impacts attributable to the stainless steel to be used for the MH compressor, mainly because of the large amount used. Considering an optimized design, with an increased alloys:steel ratio, environmental impacts of alloys for hydrogen sorption to be used in the metal hydride system become dominant. In particular the $La_{0.9}Ce_{0.1}Ni_5$ alloy shows higher impacts with respect to the $Ti_{0.95}Zr_{0.05}Mn_{1.55}V_{0.45}Fe_{0.09}$ alloy.

It must be considered that, as a possible limitation of this study, the impacts associated with the generic H₂ compressor are very likely underestimated compared to reality, because of the way the system was modeled in this study (i.e. an adaptation of an air compressor as proxy). At the same time, although the system based on metal hydrides currently does not prove to be the most suitable from an environmental point of view, it has a large room for improvement. In fact, the MH compressor has been modelled making some assumptions that probably led to an overestimation of the environmental impacts (i.e. low alloy: steel ratio and substitution of alloys over a short period of time). Taking into consideration the previous limitations and assuming a further optimization of the compressor structure, as well as the use of different alloys, with greater effectiveness than those modeled here, could allow to considerably reduce the impacts on the environment and increase the competitive advantage of this compression technology.

Results obtained in this study fill in a knowledge gap in the assessment of hydrogen value chain assessment for what concerns compression technologies, making possible to identify, in relation to a case study in defined conditions, which technology for hydrogen compression is better from an environmental and economic point of view.

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Appendix A.

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Impact category	Total	$La_{0.9}Ce_{0.1}Ni_{5}$	Ti _{0.95} Zr _{0.05} Mn _{1.55} V _{0.45} Fe _{0.09}	Stainless Steel	Metal working	Glass fibre	Pump
Climate change (x10 ² kg CO ₂ eq)	35.74	9.24	2.56	14.76	7.30	0.86	1.02
Particulate matter (x10 ^{~5} Disease inc.)	26.46	7.27	1.42	12.47	3.71	0.49	1.11
Photochemical ozone formation (kg NMVOC eq)	13.22	3.92	0.94	5.40	2.00	0.39	0.57
Acidification (mol H+ eq)	26.47	10.52	1.41	9.28	3.65	0.64	0.97
Resource use, minerals and metals (x10 ^{~3} kg Sb eq)	148.74	37.26	0.73	51.75	13.82	0.74	44.45
Resource use, energy carriers (x10 ^{^3} MJ)	43.34	11.47	3.21	16.52	9.84	1.13	1.16

 Table A.1 Numerical LCIA results for all the impact categories calculated for the production of the MH compressor.

Table A.2 Comparison of the environmental impacts associated with the compression of 1.79 kg of H_2 at 200 bar using different systems.

Impact category	MH comp	MH comp + heat NG	MH comp + grid el	MH comp + pv el	Air booster	Air booster + pv el	H₂ comp + grid el	H₂ comp + pv el
Climate change (kg CO ₂ eq)	1.77	15.47	23.05	5.37	0.16	0.07	2.82	0.73
Particulate matter (x10 ^{~8} Disease inc.)	13.08	19.27	50.38	36.58	0.61	0.54	6.77	5.15
Photochemical ozone formation (x10 ^{∿4} kg NMVOC eq)	66.93	202.25	535.40	212.70	4.16	2.63	70.65	32.57
Acidification (x10 ^{∿3} mol H⁺ eq)	14.07	28.97	108.59	35.78	0.78	0.43	13.93	5.33
Resource use, minerals and metals (x10 ^{∿5} kg Sb eq)	7.01	8.72	26.77	47.66	0.30	0.40	15.69	18.15
Resource use, energy carriers (MJ)	21.56	215.70	335.44	66.07	2.15	0.87	40.59	8.81

Table A.3 Total cost of the three systems analysed: MH compressor, air booster + air compressor and generic H_2 compressor.

System	Detail	Price	Unit of measurement
	Stainless steel	1164.24	€/unit of compressor
	Metal working	244.50	€/unit of compressor
MH compressor	$La_{0.9}Ce_{0.1}Ni_5$	10655.00	€/unit of compressor
MH - compressor	Ti _{0.95} Zr _{0.05} Mn _{1.55} V _{0.45} Fe _{0.09}	3196.00	€/unit of compressor
	Glass fibre	103.27	€/unit of compressor
	Pump	1150.00	€/unit of compressor
Air booster	Air booster	4952.00	€/unit of compressor
	Air compressor	7876.67	€/unit of compressor
Generic H ₂ compressor	Hydrogen compressor	71200.00	€/unit of compressor

Table A.4 Cost for the compression of 1.79 kg of H2, at 200 bar, with the three systems analyzed; no energy consumption was hypothesized in the case of the MH compressor, instead the use of energy from the national mix was assumed to power the system with booster and the H2 compressor.

System	Detail	Price	Unit of measurement
	Stainless steel	0.459	€/FU
	Metal working	0.085	€/FU
MH compressor	La _{0.9} Ce _{0.1} Ni ₅	7.459	€/FU
	Ti _{0.95} Zr _{0.05} Mn _{1.55} V _{0.45} Fe _{0.09}	2.237	€/FU
	Glass fibre	0.041	€/FU
	Pump	0.460	€/FU
	Air booster	1.956	€/FU
Air booster	Air compressor	0.00085	€/FU
	Electricity (Italian mix)	0.036	€/FU
Generic H ₂ compressor	Hydrogen compressor	28.124	€/FU
	Electricity (Italian mix)	0.885	€/FU

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