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COMPREHENSIVE LIFE CYCLE ANALYSIS OF DIVERSE HYDROGEN PRODUCTION ROUTES AND APPLICATION ON A HYDROGEN ENGINE

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ABSTRACT

In the effort of achieving net-zero Greenhouse Gas (GHG) emissions, hydrogen is becoming increasingly relevant in several sectors such as automotive, cogeneration, maritime, off-road, and railroad. However, hydrogen can be produced from different routes that involve different production processes and feedstocks. In contrast to the key role of hydrogen in the transport sector's decarbonization, publications that claim to address the environmental impacts of hydrogen are often focused on Global Warming Potential (GWP) and GHG emissions only. This manuscript focuses on the environmental impacts of hydrogen production considering different production routes (i.e., Steam Methane Reforming (SMR), SMR coupled with Carbon Capture and Storage (CCS), Coal Gasification (CG), CG coupled with CCS, electrolysis from fossil fuels and from wind) and a broad set of environmental impact categories, not only GWP. The Life Cycle Assessment (LCA) methodology is applied in the present study with a twofold aim. The first aim is to develop the LCA models of diverse hydrogen production routes and address present and potential well-to-tank environmental impacts. The second aim is to apply the previous findings to develop a cradle-to-grave LCA of a hydrogen engine, serving as a case study for the automotive sector. The LCA models are developed using SimaPro v.9.4.0.3 as LCA software and Ecoinvent v3.8 as background database. The functional units are 1 kg of hydrogen for the cradle-to-gate boundary and 1 mile of vehicle lifetime for the cradle-to-grave boundary. The life cycle impact assessment method is the TRACI 2.1 method developed by the US Environmental Protection Agency.

Keywords: alternative fuels, hydrogen engine, internal combustion engines, LCA, life cycle analysis.

1. INTRODUCTION

The transport sector is responsible for a large portion of Greenhouse Gas (GHG) emissions [1]. The Well-To-Wheel (WTW) phase has a significant contribution in different environmental impact categories of internal combustion engines [1], among which Global Warming Potential (GWP). For this reason, alternative solutions are under investigation, such as hydrogen combustion engines (H2-ICEs) and fuel cells (FCs).

Hydrogen is becoming more important as a carbon-free energy carrier that can significantly contribute to the process of reducing carbon emissions. In terms of hydrogen donors, hydrogen can be extracted from fossil fuels, biomass, or water

[2]. However, natural gas, which mostly consists of methane, various hydrocarbons and CO₂, is currently the most used source [2,3]. In terms of production routes, hydrogen can be produced through dedicated routes (e.g., reforming, gasification) or as a by-product or co-product (e.g., catalytic reforming [4], chloro-alkali electrolysis process [2]). A minor role in hydrogen production is played by electrolysis, where water is split into hydrogen and oxygen by the electric current that is applied by cathodes and anodes [2,5]. Concerning reforming, actually three methods exist: steam reforming (using water as an oxidant and a source of hydrogen), partial oxidation (using oxygen in the air as the oxidant), or a combination of both called autothermal reforming [2]. Steam reforming is used to extract hydrogen from natural gas and less frequently from liquid petroleum and naphtha, while partial oxidation is used to extract hydrogen from heavy fuel oil and coal. [2]. For gasification the raw materials are usually coal or biomass [2]. For water electrolysis, currently, water can be split by alkaline electrolysis (AE), proton exchange membrane electrolysis, solid oxide electrolyser cell electrolysis, anion exchange membrane electrolysis [6].

Despite the increasing relevance of hydrogen, the environmental consequences of various hydrogen production processes are often disregarded, especially for environmental indicators other than GWP (e.g., acidification, eutrophication). In fact, considering the pressing demand for low-carbon hydrogen, it is crucial to verify that the environmental impact is not shifted elsewhere [6]. According to [7], carbon sequestration reduces the GWP of hydrogen produced through coal gasification (CG) by 44%, but at the same time it raises the impacts in terms of acidification, eutrophication, and abiotic depletion.

The aim of the present study is to give a clear and comprehensive evaluation of the WTT contribution in hydrogen-fueled vehicles, with a specific focus on H2-ICE vehicles rather than FCs. To do so, (1) a literature review focused on hydrogen Life Cycle Assessment (LCA) studies has been conducted to develop the LCA models of diverse hydrogen production routes and address present and potential WTT environmental impacts, and (2) the LCA approach has been used to evaluate the environmental impacts of an H2-ICE. Compared to conventional internal combustion engines, hydrogen engines have significantly lower Tank-To-Wheel (TTW) contribution, in terms of GHG emissions. In fact, hydrogen does not contain carbon and, therefore, H2-ICEs do not emit carbon monoxide or

carbon dioxide during operation. Despite H₂-ICEs may have other emissions during operation (i.e., nitrogen oxides, unburned hydrocarbons, and particulate matter), their main driver to the WTW impact is the Well-To-Tank (WTT) contribution. The WTT contribution comprises the emissions related to hydrogen production which differ based on the assumed production route.

Among the global initiatives on this topic, in 2011, two guidance documents (FC-Hy Guide) for performing LCAs on fuel cells and hydrogen production systems valid for the European geographical scope have been published [4,8]. In these documents, it is highlighted the importance of ensuring comparability by defining consistent system boundary and functional unit if diverse hydrogen production routes are put in comparison. Additionally, two WTT assessment initiatives, grounded on the LCA methodology, can be remarked in Europe (EU) and the United States (US). In EU, the JEC WTT Report v5 [9] comprises a WTT contribution modeled in the Environmental Footprint (EF) database [10], which reports the energy demand and the related GHG emissions of producing, and distributing several fuels suitable for road transportation, and a TTT contribution, which estimates the energy consumption and related GHG emissions of a vehicle concept using the AVL Cruise™ [11] simulation tool [12]. In the US, an LCA tool called Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET®) [13] estimates the WTT as well as the full life cycle of vehicles [12].

2. MATERIALS AND METHODS

2.1 Literature review

In this study, a literature review focused on hydrogen LCAs and covering the period 2015-2024 has been conducted to address the environmental impacts of diverse production routes. The search was carried out in Scopus using the keywords “hydrogen” and “LCA”. Articles have been excluded if they do not feature a full LCA or even a GWP assessment. A total of 173 publications have been found, corresponding to a total of 452 scenarios for hydrogen production. Then, among the 173 publications found, those publications that were not replicable in terms of LCA model development have been excluded. Replicability has been chosen as a high-relevant feature because, according to [6], 36% of the studies published between 2015-2022 used an LCIA method that was at least ten years old. This is important because our comprehension of the impact of various emissions has been improved over time. This search gave a final cohort of 103 studies, corresponding to 276 scenarios for hydrogen production. At this point, 5 scenarios have been identified that differ per hydrogen production route and energy source aiming to depict the current main production routes. Then, each publication has been scored based on three factors: (1) publication year, (2) accuracy, and (3) quality of data sources. Accuracy has been scored based on the percentage difference between the declared GWP result and the average GWP calculated for each production route (Fig. 3, Tab. 2). Lastly, for each hydrogen production route, one publication has been identified as the most reliable source of data, serving as a starting point for the LCA models of the WTT contributions.

2.2 LCA methodology

The LCA methodology evaluates the environmental impacts associated with a product by compiling an inventory of relevant input and output material and energy flows exchanged by the product system with the environment and the technosphere and interpreting the results according to the objectives of the study. This study was performed according to international standards, ISO 14040 and ISO 14044 [14,15]. Also, this study refers to the guidelines of the FC-Hy Guide [4,8]. To avoid biased LCA results, the methodology applied includes the following stages:

- Goal and scope definition. The term “goal” refers to clearly stating the study’s goal. ISO standards 14040 and 14044 [14,15] define “scope” as the set of assumptions needed to achieve the goal (i.e., system boundary, functional unit, product/s under study, data sources, geographical coverage, impact assessment method, allocation approach if any).
- Life Cycle Inventory (LCI), in which all the input and output flows that fall within the system boundaries are collected.
- Life Cycle Impact Assessment (LCIA), conducted according to the chosen impact assessment method.
- Result interpretation.

2.2.1 Goal and scope definition

The aim of the present work is twofold: (1) to develop the LCA models of diverse hydrogen production routes and address present and potential cradle-to-gate environmental impacts by means of a literature review, (2) to develop a cradle-to-grave LCA of a hydrogen engine redesigned from a diesel engine, serving as a case study for the automotive sector. The geographical scope of this study is the US. The system boundaries are cradle-to-gate for hydrogen production and cradle-to-grave for the full LCA of the H₂-ICE. The cradle-to-gate boundary (Fig. 1) comprises feedstock acquisition and transport, electricity production and distribution, conditioning (e.g., sulfur removal, feedstock compression and heating), conversion (e.g., reforming, gasification, electrolysis), purification (e.g., through pressure swing adsorption (PSA), membrane purifiers), conditioning (e.g., compression, liquefaction, odorization), transport and compression at refueling station. In fact, after hydrogen is produced in the conversion step, it undergoes a purification step, determined mainly by its intended end use [2,4]. In all cases, a synthesis gas is produced and subsequently purified if pure hydrogen is needed [2]. A high purity hydrogen of at least 99.97-99.99% is needed for FC electric vehicles [6]. Then, depending on the demand and distance, hydrogen can be distributed by means of tube trailers, liquid tankers or pipelines [16]. The type of distribution also influences the conditioning because, for instance, hydrogen is often odorized for pipeline transportation [4] and compression pressure may differ based on the distribution mean [16]. Lastly, hydrogen must be delivered to refueling stations at 350-700 bar. The cradle-to-grave boundary (Fig. 2) comprises raw material acquisition and preprocessing, manufacturing of supplier components, transport of raw materials and supplier components, engine manufacturing, additional materials and

processing for H2-ICE redesign, engine distribution, WTT, TTW and maintenance emissions during use, and End-of-Life (EoL). The functional units are 1 kg of hydrogen for the cradle-to-gate boundary, and 1 driven mile of the vehicle lifetime for the cradle-to-grave boundary. The vehicle lifetime is assumed to be 150,000 miles in compliance with [17]. The LCA models have been developed using SimaPro v.9.4.0.3 [18] as LCA software and Ecoinvent v3.8 [19] as background database. The life cycle impact assessment method is the TRACI 2.1 method [20] developed by the U.S. Environmental Protection Agency.

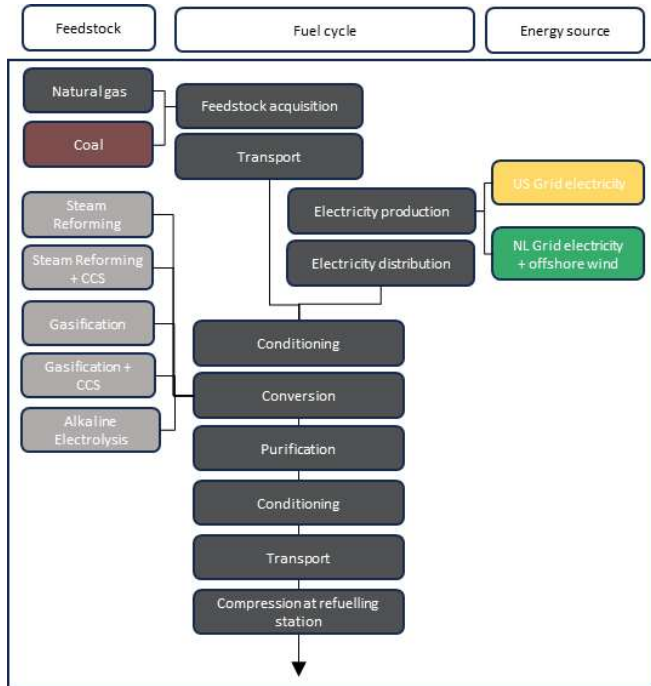


FIGURE 1: CRADLE-TO-GATE SYSTEM BOUNDARY.

2.2.2 Life Cycle Inventories

2.2.2.1 Well-To-Tank

Seven scenarios have been identified in this work (Fig. 1-2) as summarized hereafter:

- DIE-ICE
- H2-ICE through SMR
- H2-ICE through SMR with CCS
- H2-ICE through CG route
- H2-ICE through CG with CCS
- H2-ICE through AE and wind-based electricity
- H2-ICE through AE and fossil-based electricity

Those processes in which hydrogen is produced as by-product or at low Technology Readiness Level (TRL) have been discarded. Considering the global dedicated routes, approximately 96% of hydrogen is produced through SMR or CG [6]. Instead, AE has been assumed, because of the great attention devoted to electrolysis of water using renewable energy [6]. Because, it may be a promising strategy, two scenarios coupling SMR and CG with Carbon Capture and Storage (CCS)

have been considered. Lastly, the hydrogen scenarios have been compared with a diesel scenario (DIE-ICE).

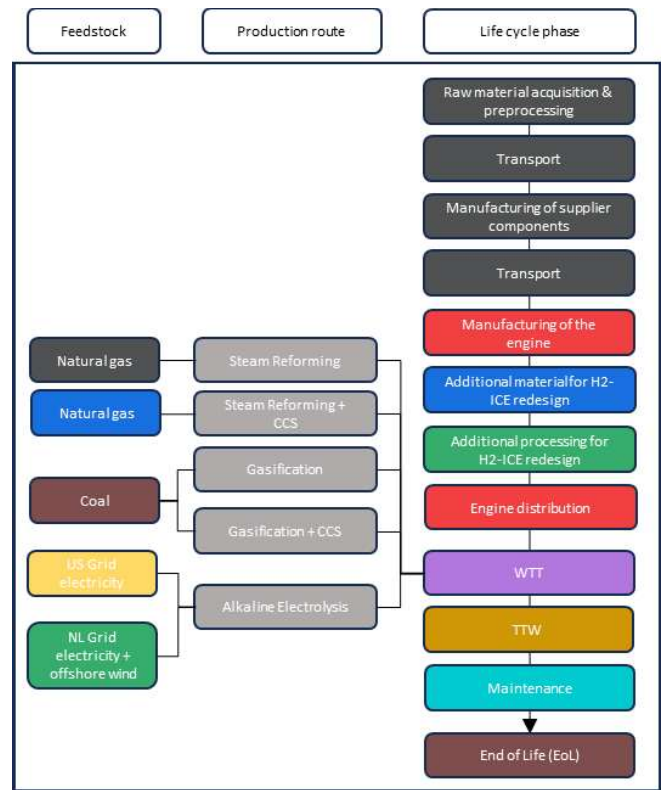


FIGURE 2: CRADLE-TO-GRAVE SYSTEM BOUNDARY.

Steam methane reforming

This work refers to [21] for hydrogen production through conventional SMR. Hydrogen has been assumed to be produced in a large-scale central plant. The fuel cycle adopted in [21] includes natural gas extraction and supply, conditioning (i.e., the feedstock is compressed and heated), steam reforming (i.e., CH₄ and steam react to produce CO and H₂), water gas shift (WGS) (i.e., additional H₂ is produced during the reaction of CO and steam), purification of syngas by means of a PSA unit, and cooling [21,22]. Hydrogen is the only output product of the process, therefore there has been no need for allocation. Capital goods (machinery, equipment, and buildings) are excluded from the system boundary. The obtained hydrogen has 22 bar pressure, 40°C temperature, and 99.9% purity. With respect to [21], the US electricity mix has been assumed for electricity production, adopting the inventory data available in the Ecoinvent database. To consider hydrogen compression before distribution, an extra load of 0.6 kWh/kg H₂ has been taken into account in compliance with [16] in order to compress the hydrogen from 22 bar to 200-250 bar and ensure comparability with the other routes. Hydrogen has been assumed to be distributed in gaseous form by means of tube trailers, which have been modelled adopting the 16-32 metric ton freight lorry dataset fulfilling the EURO 6 emission standards available on Ecoinvent database. An average distance of 200 miles has been assumed

considering the locations of the refueling stations (in 2023, there were 59 open retail hydrogen stations in the US, most of them in California) [23] and the locations of the main hydrogen producers in California based on [24]. Lastly, for final compression at the refueling station, an additional 2.4 kWh/kg H₂ has been considered based on [24] to compress it to 800 bar.

Steam methane reforming with CCS

This work refers to [22] for hydrogen production through SMR with CCS. This system is multifunctional because it produces both hydrogen and carbon dioxide. To solve multifunctionality, 100% of the environmental burdens have been allocated to hydrogen, being the main product of the system. Hydrogen has been assumed to be produced in a large-scale central plant with a production volume of 216 tons.day⁻¹ [22]. The fuel cycle includes feedstock extraction and supply, conditioning (i.e., the feedstock is compressed and heated), steam reforming, WGS, CO₂ capture, an additional methanation stage to further reduce the CO content, the purification of syngas through a PSA unit, conditioning (i.e., compression using a four-stage compression train), and transport to the end user. Whenever applicable, direct heat exchange of process streams has been exploited as the energy source. The obtained hydrogen has 200 bar pressure, which is already suitable for compressed hydrogen tube trailers, 333 K temperature, liquid state and 99.5% purity. Contrarily to [22], emissions related to plant construction have been excluded to ensure comparability among all routes. The US electricity mix has been assumed for electricity production, adopting the inventory data available in the Ecoinvent database. Instead of the original dataset for feedstock supply and transport available in [22], natural gas has been assumed to be supplied as high-pressure gas (>1 bar) through pipelines adopting the US geography available on the Ecoinvent database. Hydrogen has been assumed to be distributed by means of tube trailers, and to be compressed to 800 bar at the refueling station, as in the SMR route.

Coal gasification

For hydrogen production through CG, this work is based on [3]. In this route, coal is partially oxidized in the presence of oxygen or air to produce syngas that comprises CO, H₂, CO₂, and unreacted CH₄ [3]. Then, additional hydrogen is produced by means of the WGS. The obtained hydrogen has 30 bar pressure and 99.99% purity. The US electricity mix has been assumed for electricity production, adopting the inventory data available in the Ecoinvent database. Hydrogen has been assumed to be distributed by means of tube trailers, and to be compressed to 800 bar at the refueling station, as in the SMR route.

Coal gasification with CCS

For hydrogen production through CG with CCS, this work refers to [3] as in the CG route. This system is multifunctional as it produces both hydrogen and carbon dioxide. To solve multifunctionality, 100% of the environmental burdens are allocated to hydrogen, being the main product of the system.

Alkaline electrolysis

For hydrogen production through AE, this work refers to [25]. The fuel cycle adopted in [25] comprises the acquisition of raw materials (i.e., mining, processing, and transport), the manufacturing of the electrolyzer system components, and the production of the electricity consumed during the electrolysis process. During electrolysis, oxygen is produced along with hydrogen as a by-product, but it is currently venting into the atmosphere and not being reintroduced in the market [25], therefore there has been no need for allocation. According to [6], this approach is commonly shared among LCAs focused on electrolysis. The obtained hydrogen has 30 bar pressure, but purity is not declared. Nevertheless, [6] stated that electrolytic techniques can achieve a hydrogen purity of 99.9% without requiring any additional purification step, therefore, a high-purity product has been assumed. Hydrogen has been assumed to be distributed by means of tube trailers and to be compressed to 800 bar at the refueling station, as in the SMR and CG routes.

Two alkaline electrolysis scenarios have been set up: one based on the original electricity mix of [25], which is a mix of the electricity mix of the Netherlands (NL) (3.9%) and offshore wind electricity (96.1%), and the other based on the 2019 US electricity mix. The former represents a green electricity mix, while the latter represents a fossil-based electricity mix. In fact, in 2019, the US mix consisted of 62% fossil sources. The different electricity mixes have been incorporated at that point in the life cycle in which grid electricity is supplied to operate the electrolyzer. The fuel share in the electricity mixes for both AE scenarios can be found in Tab. 1. The inventory data in the Ecoinvent database assumed for offshore wind in the Netherlands refers to 1–3 MW offshore wind turbines.

TABLE 1: FUEL SHARE IN ELECTRICITY MIXES IN THE AE SCENARIOS

| | AE NL | AE US |
|-------------|-------|-------|
| Wind | 96.7% | 7.24% |
| Natural Gas | 1.49% | 38.4% |
| Nuclear | 0.26% | 20.1% |
| Hard Coal | 1.02% | 13.6% |
| Lignite | 0.19% | 10.1% |
| Hydro | 0.17% | 7.69% |
| Other | 0.23% | 2.72% |

2.2.2.2 Tank-To-Wheel

For what concerns the TTW emissions, the engine is assumed to be mounted on a heavy-duty pickup truck belonging to the 2b class of the Environmental Protection Agency (EPA) vehicle classification in compliance with [26]. Fuel consumption has been evaluated through an ad hoc simulation model. The cycle tests of the Federal Test Procedure (FTP) and the Highway Fuel Economy Test (HFET) weighted at 55% and 45%, respectively, have been used as reference cycles to estimate the trend of engine Brake Mean Effective Pressure (BMEP) and engine speed over the course of a typical driving mission. Coast-down coefficients have been assumed based on [27], while a typical shift curve has been hypothesized as a function of speed. Integrating the evolution over time of the engine operating point

with the Brake Specific Fuel Consumption (BSFC), it has been possible to estimate the overall fuel consumption. For estimating CO₂ and pollutant emissions, a simulation model like the one used to assess fuel consumption has been used, adopting the FTP cycle only. Non-exhaust emissions have been estimated by means of emission factors for pickup trucks based on [28].

Concerning maintenance, data have been retrieved from the maintenance handbook developed for the DIE-ICE vehicle under study. The maintenance emissions of both DIE-ICE and H₂-ICE comprise the consumption of lubricating oil, water, ethylene-glycol, and polyester along the entire life cycle of the two engines. With respect to the DIE-ICE, in the H₂-ICE, the use of a different lubricating oil and the substitution of spark plugs have been considered. Neither engine replacement during the vehicle lifetime nor extraordinary maintenance have been considered in this study.

2.2.2.3 Engine production and EoL

Lastly, for the production and EoL emissions of the hydrogen engine, a diesel engine redesigned to run on hydrogen has been considered based on [29,30]. It is a monofuel engine suitable for pickup trucks, with 8 cylinders arranged on two V-shaped banks, 922 lb weight, total displacement of 6.6 liters, 910 lb-ft maximum torque and 445 Hp rated power. The engine has been assumed to be manufactured and re-designed in the US, while supplier components are supplied from different locations in the world.

3 RESULTS AND DISCUSSION

As shown in Fig. 3 and Tab. 2, according to the analyzed hydrogen LCAs available in the literature [1,3,21,22,31–47], it has been found that producing 1 kg of hydrogen has an average GWP of 10.4 kg CO_{2eq}. Similar graphs have been obtained for the other production routes and the average results and standard deviations are reported in Tab. 2. Results are given per kg of hydrogen. It has been assumed 120 MJ/kg as the hydrogen lower heating value. High deviations from the average values have been found for those production technologies involving CCS, especially CG, due to the low number of samples, and for AE due to the widespread results among the samples.

Figure 4 shows the GWP results obtained in this study for the WTT contribution, varying hydrogen production scenario.

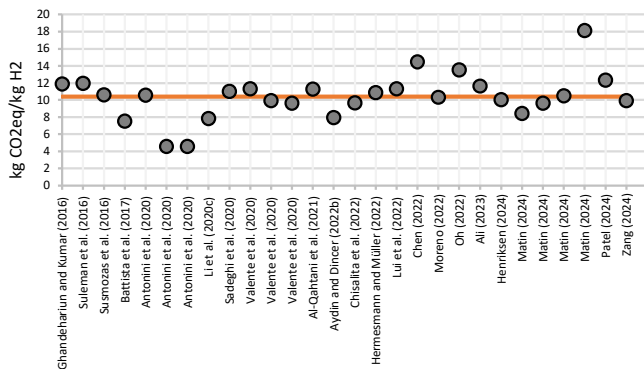


FIGURE 3: SPREAD OF LITERATURE GWP RESULTS OF HYDROGEN PRODUCTION THROUGH SMR.

TABLE 2: AVERAGE GWP RESULTS FROM 2015 TO 2024 BASED ON THE LITERATURE

| Production route | N. papers | Average GWP (kg CO _{2eq} /kg H ₂) | Standard deviation (kg CO _{2eq} /kg H ₂) |
|------------------|-----------|--|---|
| SMR | 28 | 10.4 | 2.6 |
| SMR + CCS | 8 | 4.28 | 1.8 |
| CG | 9 | 26.0 | 11.0 |
| CG + CCS | 3 | 11.1 | 6.4 |
| AE | 26 | 8.86 | 11.3 |

In the SMR scenario, the GWP is 16 kg CO_{2eq}/kg H₂. The main contributor is the conversion step mainly because of the direct emissions to air. In the SMR + CCS scenario, the GWP is 14.7 kg CO_{2eq}/kg H₂. In this case the contribution of the conversion step decreases and the overall GWP is reduced by 8.1% with respect to the SMR scenario. This low reduction is mainly due to the higher energy consumption in the SMR + CCS related to the capture process itself. Moreover, in LCA, the modelling of captured CO₂ depends on its intended use/disposal. We assumed to not resell the captured CO₂, thus no additional benefit aside from the reduced emission of CO₂ is considered in this study. In the CG scenario, the GWP jumps to 28.9 kg CO_{2eq}/kg H₂. Also in this case, the main contributor to this impact is the conversion step mainly because of the direct emissions to air. In the CG + CCS scenario, the GWP is 10.8 kg CO_{2eq}/kg H₂. In this case the contribution of the conversion step decreases and the overall GWP is reduced by 62.6% with respect to the CG scenario. In the AE NL scenario, the GWP drops to 3.67 kg CO_{2eq}/kg H₂. In fact, in this case the hydrogen production process significantly benefits from the green electricity mix, which is primarily comprised of offshore wind-generated electricity. In this route, the additional compression steps (magenta and light blue contributions) acquire relevance with respect to the overall GWP impact. In the AE US scenario, the GWP ramp up to 27.2 kg CO_{2eq}/kg H₂. The GWP rise in the AE US scenario is due to the electricity mix as both the AE scenarios are based on the same hydrogen production process but vary only in the electricity mix adopted. Lastly, results obtained in this study may differ from the average GWP results found in the literature (Tab. 2) because of the different assumptions between LCA studies (e.g., different TRL, LCIA method, system boundary). This issue has also been raised by [6], that urges researchers to enhance comparability of their results.

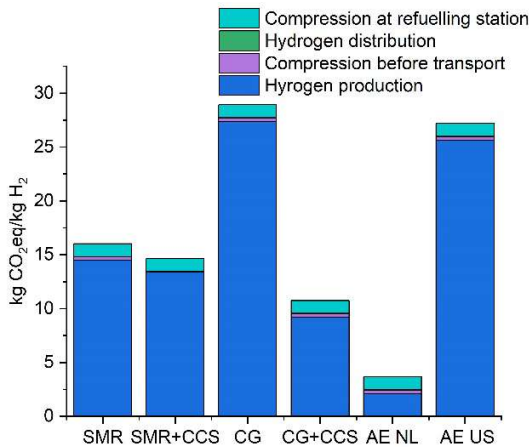


FIGURE 4: GWP RESULTS OF WTT CONTRIBUTION.

Figure 5 shows a more comprehensive comparison of the results of hydrogen production. In compliance with the TRACI method, nine additional impacts besides GWP have been investigated. As in the GWP results (Fig. 4), the AE NL scenario (dark blue bars) has the lowest impact in the categories of smog formation, acidification, eutrophication, non carcinogenics, respiratory effects, and fossil fuel depletion. Contrarily to the GWP results, the worst scenario is the AE US scenario (light blue bars) in the categories of smog formation, acidification, carcinogenics, and respiratory effects. The reason is the adoption of the US electricity mix. Also, the SMR scenario (dark green bars) is the worst in the categories of eutrophication and non carcinogenics. The reason is the plant wastewater treatment for both. Lastly, the SMR + CCS scenario (light green bars) is the worst in ozone depletion and fossil fuel depletion. The reason is natural gas extraction and supply. In compliance with [7], CG + CCS (yellow bars) significantly reduces the GWP of hydrogen produced through CG, but at the same time it raises the impacts in terms of acidification and eutrophication. The same can be observed for SMR + CCS (light green bars) because CCS does not significantly reduce the GWP impact of hydrogen produced through SMR, but at the same time it raises the impacts in terms of ozone depletion, smog formation, acidification, respiratory effects, and fossil fuel depletion.

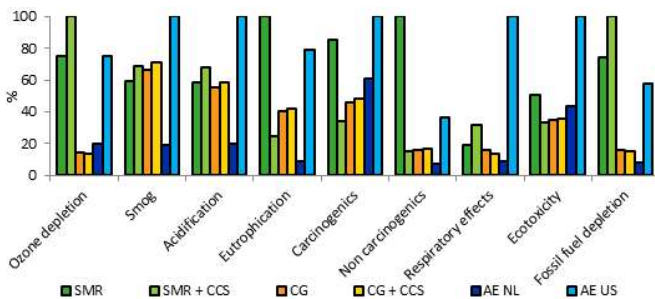


FIGURE 5: LCA RESULTS OF WTT CONTRIBUTION.

Figure 6 shows the comparison of the GWP results related to the full LCA of the DIE-ICE and H2-ICE under study, by varying WTT scenario. The baseline DIE-ICE scenario accounts for 0.586 kg CO_{2eq}/FU. The impact is primarily due to the TTW

contribution (80.7 %) and WTT contribution (15.7 %). The H2-ICE SMR scenario accounts for 0.848 kg CO_{2eq}/FU while the H2-ICE SMR + CCS scenario accounts for 0.777 kg CO_{2eq}/FU. The H2-ICE CG scenario accounts for 1.51 kg CO_{2eq}/FU while the H2-ICE CG + CCS scenario accounts for 0.577 kg CO_{2eq}/FU. Lastly, the H2-ICE AE NL scenario accounts for 0.213 kg CO_{2eq}/FU while the H2-ICE AE US scenario accounts for 1.42 kg CO_{2eq}/FU. The H2-ICE scenarios are primarily influenced by the WTT contribution. The H2-ICE AE NL scenario, which counts on a wind-based electricity mix, resulted as the most favorable among the H2-ICE scenarios and showed a decrease of -63.7% compared to the baseline DIE-ICE scenario.

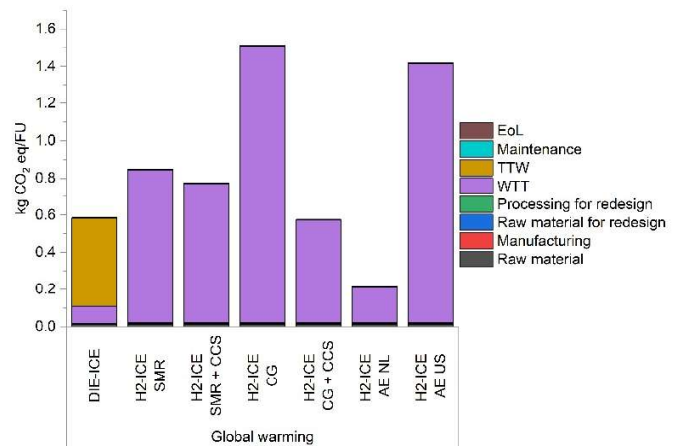


FIGURE 6: GWP RESULTS OF THE FULL LIFE CYCLE.

Figure 7 shows the LCA results of the full life cycle of the engines under study. In compliance with the TRACI method, the impacts of ozone depletion, fossil fuel depletion, eutrophication, ecotoxicity, carcinogenics, non carcinogenics, acidification, respiratory effects, and smog formation have been calculated. In all the investigated categories, the impacts are primarily driven by the WTT contribution in the H2-ICE scenarios. The same occurs in the majority of the impact categories in the case of the DIE-ICE scenario with exception of ecotoxicity, which is driven by the EoL phase for 81.8 % due to aluminum scrap treatment; carcinogenics, which is driven by the engine's raw materials (mainly cast iron and steel used in the block, crank rotating and aftertreatment systems) for 75.8 %; and smog formation, which is driven by the TTW contribution by 70.3 % due to the emission of NO_x during use. Diesel production and supply is also the main driver for the DIE-ICE scenario in ozone depletion (accounting for 97.1 % of the overall impact), fossil fuel depletion (97.7 %), eutrophication (68.6 %), acidification (55.8 %), and respiratory effects (52 %).

For ozone depletion, natural gas production and supply are the main drivers for the H2-ICE SMR (accounting for 84.4 %) and H2-ICE SMR + CCS scenarios (72.7 %). Hard coal is the main driver of the H2-ICE CG (39.7 %) and H2-ICE CG + CCS scenarios (47.9 %). The production of the AE stack materials is the main driver of the H2-ICE AE NL scenario (53.2 %) mainly

due to tetrafluoroethylene production. The US electricity mix is the main driver of the H2-ICE AE US scenario (80.4 %).

For fossil fuel depletion, natural gas production and supply are the main drivers for the H2-ICE SMR (90.5 %) and SMR + CCS scenarios (76.4 %). Hard coal is the main driver of the H2-ICE CG (52.7 %) and H2-ICE CG + CCS scenarios (62.5 %). Compression at refueling station (28 %) and NL electricity mix (27.3 %) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (97 %).

For eutrophication, the plant waste treatment (91.9 %) is the main driver for the H2-ICE SMR scenario while US electricity mix is the main driver of the H2-ICE SMR + CCS scenario (78.9 %). Hard coal is the main driver of the H2-ICE CG (75.5 %) and H2-ICE CG + CCS scenario (82.6 %). Compression at refueling station (35.3 %) and NL electricity mix (23.1 %) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (97.9 %).

For ecotoxicity, plant waste treatment (44.7 %) as well as aluminum treatment during EoL phase (29.6 %) are the main drivers for the H2-ICE SMR scenario. The US electricity mix as well as aluminum scrap treatment during EoL phase are the main drivers for the H2-ICE SMR + CCS scenario (34.6 % and 36.8 %, respectively). Hard coal as well as aluminum scrap treatment during the EoL phase are the main drivers of the H2-ICE CG (33.7 % and 35.7 %, respectively) and H2-ICE CG + CCS scenario (38.2 % and 35.5 %, respectively). Treatment of aluminum scrap during EoL phase (32.1 %) and NL electricity mix (34.9 %) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (68.1 %).

For carcinogenics, plant waste treatment (70.2 %) is the main driver for the H2-ICE SMR scenario. The US electricity mix is the main driver for the H2-ICE SMR + CCS scenario (40.7 %). Hard coal is the main driver of the H2-ICE CG (55.3 %) and H2-ICE CG + CCS scenarios (60.3 %). The production of the AE stack materials (19.8 %) and the NL electricity mix (45.5 %) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (70 %).

For non carcinogenics, plant waste treatment (94.6 %) is the main driver for the H2-ICE SMR scenario. The US electricity mix is the main driver for the H2-ICE SMR + CCS scenario (55.6 %). Hard coal is the main driver of the H2-ICE CG (78.8 %) and H2-ICE CG + CCS scenarios (74 %). Compression at refueling station (17 %) and NL electricity mix (34.7 %) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (92.5 %).

For acidification, plant waste treatment (56.9 %) is the main driver for the H2-ICE SMR scenario. Auxiliary steam is the main driver for the H2-ICE SMR + CCS scenario (41.7 %). Hard coal

is the main driver of the H2-ICE CG (72.8 %) and H2-ICE CG + CCS scenarios (78.9 %). Compression at refueling station (16.4 %), NL electricity mix (21 %) and AE stack materials (24.7 %) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (88.5 %). For respiratory effects, plant waste treatment (45 %) is the main driver for the H2-ICE SMR scenario. The US electricity mix is the main driver for the H2-ICE SMR + CCS scenario (76.2 %). Hard coal and compression at refueling station are the main drivers of the H2-ICE CG (25.5 % and 24.5 %, respectively) and H2-ICE CG + CCS scenarios (34.1 % and 28.8 %, respectively). Compression at refueling station (40.6%) and NL electricity mix (30.6%) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (97.1 %).

For smog formation, plant waste treatment (53 %) is the main driver for the H2-ICE SMR scenario. Auxiliary steam is the main driver for the H2-ICE SMR + CCS scenario (38.6 %). Hard coal is the main driver of the H2-ICE CG (68.4 %) and H2-ICE CG + CCS scenarios (73.7 %). Compression at refueling station (13.2 %) and NL electricity mix (40 %) are the main drivers of the H2-ICE AE NL scenario. The US electricity mix is the main driver of the H2-ICE AE US scenario (85.6 %).

CONCLUSION

Hydrogen can be essential in achieving environmental objectives. However, the outcome depends on the underlying energy source and the specific conversion method employed for hydrogen production. The present study has investigated the comprehensive environmental impacts of hydrogen production considering the current main production routes and the available publications on this topic from 2015 to 2024. US geography has been assumed, and a wide range of impact categories has been evaluated. Then, results have been exploited to estimate the life cycle environmental impacts of an H2-ICE against a DIE-ICE, both assumed to be mounted on pickup trucks.

It has been found that current literature LCA studies on hydrogen production may be biased 1) if the focus is solely on GWP, because authors may have not collected data on substances responsible for emissions other than GWP, 2) if the source of data is not primary or data have not been validated, in fact available and replicable publications have been found to be largely based on process simulations rather than on primary data from existent hydrogen production plants, 3) when it comes to compare diverse hydrogen production techniques because the available publications are often based on different assumptions (e.g., different TRL, LCIA method, system boundary), or they are not transparent in declaring them, or they are not replicable. In fact, when diverse hydrogen production routes must be compared, it is necessary to ensure comparability by adopting the same system boundary and functional unit.

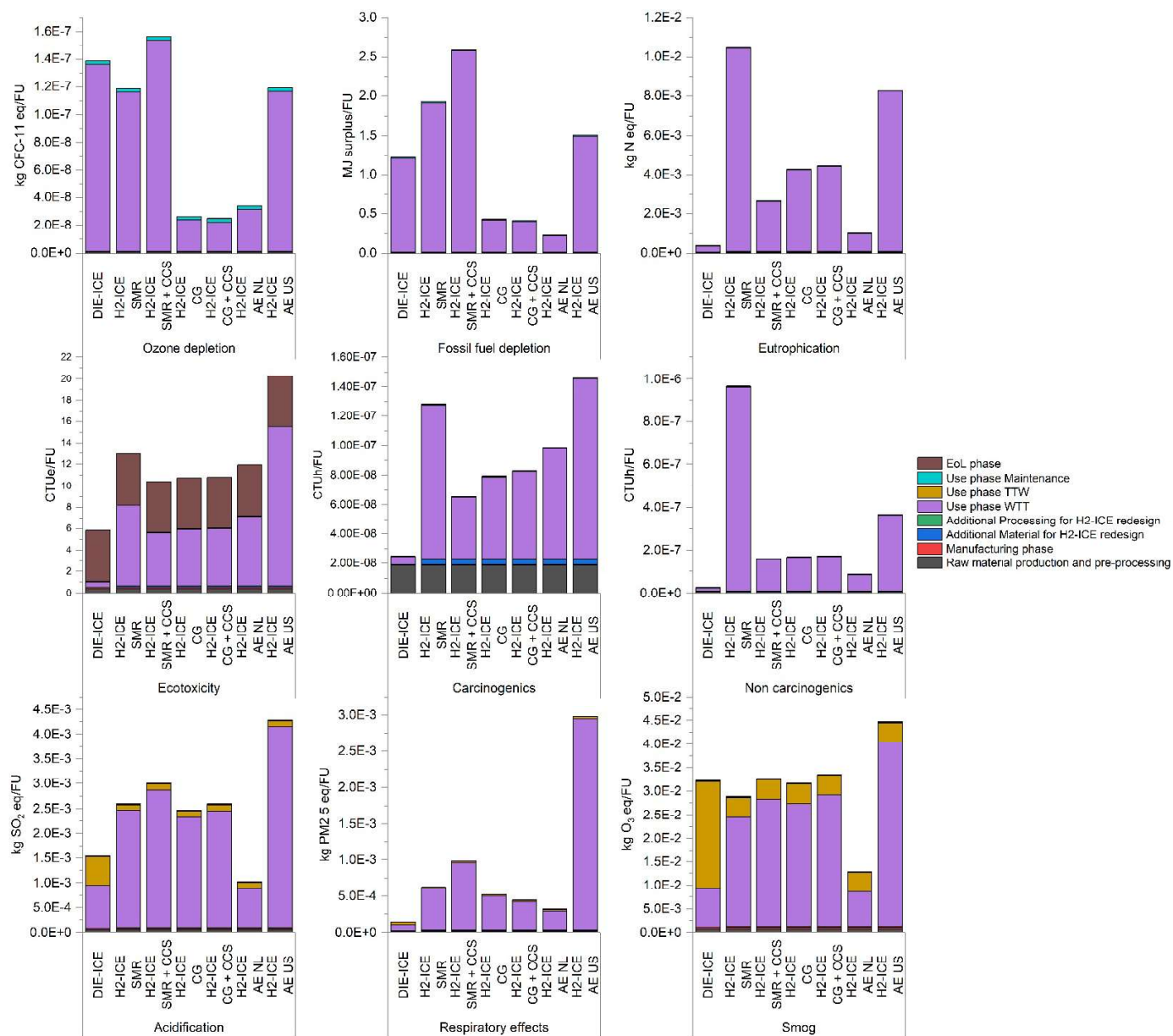


FIGURE 7: COMPARISON OF COMPREHENSIVE LCA RESULTS FOR THE FULL LIFE CYCLE.

Also, diverse hydrogen products exist that vary by state (gaseous, liquid), temperature, pressure, and purity. Moreover, plants may vary in terms of TRL and production volumes and LCA studies may include or not the emissions related to infrastructure construction (which are noted to be negligible in most of the production routes except for nuclear-based energy). Lastly, the LCIA method and version must be consistent among the routes.

In the present study, all the available publications have been scored in terms of publication year, accuracy, and data quality to select those data sources that better depict the production routes under study. Then, to ensure comparability, the system boundary and the functional unit have been harmonized when necessary to

include all the steps from feedstock acquisition to hydrogen compression at refueling station and to compare the results adopting the same functional unit, i.e., 1 kg hydrogen.

In terms of GWP and WTT, the wind-based electrolysis scenario, called AE NL scenario, resulted as the least impactful, thus alkaline electrolysis has been found to be the best solution but only with the adoption of a low-carbon electricity mix. Also, in terms of other impact categories, the AE NL scenario has the lowest impact in the categories of smog formation, acidification, eutrophication, non carcinogenics, respiratory effects, and fossil fuel depletion. Instead, the 2019 US electricity mix is the primary reason why the AE US scenario does not bring the same benefits as the AE NL scenario, and it is even the worst scenario if smog

formation, acidification, carcinogenics, and respiratory effects are considered.

In terms of GWP and full LCA, the results fully align with the WTT results, being the H2-ICE AE NL scenario the least impactful with a reduction against the DIE-ICE of 63.7 % throughout the entire life cycle. Potential improvements exist for the investigated hydrogen routes. For H2-ICE SMR + CCS, the adoption of a greener electricity mix may further decrease the impacts of global warming, ecotoxicity, carcinogenics, and respiratory effects, while avoiding the need of additional steam during the process may reduce the impacts of acidification and smog formation. Also, for the H2-ICE CG + CCS scenario, the adoption of a greener electricity mix may further reduce the impacts of ozone depletion, fossil fuel depletion, eutrophication, carcinogenics, respiratory effects. Moreover, the use of lignite coal instead of bituminous coal should be investigated. Reducing the impact or the use of AE stack may be beneficial for the H2-ICE AE NL scenario and reduce the impacts of ozone depletion, carcinogenics and acidification. While for H2-ICE AE US, a future and greener electricity mix should be investigated. Moreover, other alternative low-carbon methods should be investigated, but opportunely scaled to ensure comparability with the current methods in terms of TRL. Lastly, the environmental assessment should be coupled with an economic assessment because currently the lowest GWPs are achieved by the more expensive production methods.

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