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Climate impact of hydrogen as fuel for the heavy road transportation: A time-dependent life cycle methodology based assessment

- *Klimatpåverkan av vätgas som bränsle för tunga fordon i vägtrafiken: En tidsberoende livscykelmetod baserad analys*

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Abstract

Currently, the transportation sector stands for one third of all greenhouse gas emissions in Sweden. Hydrogen (H_2) could contribute to a decarbonized transportation sector since water is the only direct emission from a fuel cell electric vehicle. The higher energy density of H_2 compared to batteries makes H_2 better in a zero-emission system for heavy truck vehicles and long-distance transportations. Depending on the different production processes, the climate impact of H_2 varies, which encourages a life cycle assessment (LCA) based methodology. The production processes of H_2 are commonly referred to as colours, in which H_2 from steam methane reforming (SMR) with natural gas as feedstock is known as 'grey H_2'. Further, if carbon capture and storage (CCS) is added, it is referred to as 'blue H_2'. There is a possibility to replace natural gas with biomethane as feedstock, which in this study is referred to as 'beige H_2', and with CCS it can be called 'orange H_2'. Another production technology is through water-electrolysis from renewable electricity, which is referred to as 'green H_2'.

The chosen climate metrics for the LCA study are the global warming potential (GWP) and the absolute global temperature potential (AGTP). The GWP of a heavy fuel cell truck is between 2% to 110% lower than for a conventional diesel truck. Grey H_2 contributes with the highest CO_2-equivalent emissions and orange H_2 contributes with the lowest. To assess the AGTP, different future scenarios were elaborated with H_2 implementation as diesel displacement for heavy truck transportation. The future scenarios have different mixes of H_2 colours based on future market trends. Depending on the mix of H_2 colours, the temperature increase varies from $1.6 \cdot 10^{-15}$ to $1.8 \cdot 10^{-15}$ K/tonne-km, which corresponds to a temperature reduction between 9% to 21% compared to heavy truck transport with only diesel. To reach the Swedish national target of net-zero emissions by 2045, a higher share of renewable fuels together with H_2 is most likely necessary.

Keywords: hydrogen production, steam methane reforming, carbon capture and storage, water-electrolysis, heavy trucks

Executive summary

Currently, the transportation sector stands for one third of all greenhouse gas emissions in Sweden. To reach the Swedish national target of net-zero emissions by 2045, a larger share of renewable fuels must be implemented. In a future decarbonized transportation sector, hydrogen (H_2) has been proposed to play a major role as it can be used for heavy truck transport, where battery electric vehicles are less beneficial.

Even though water is the only direct emission from H_2, the climate impact from the production processes varies. Hydrogen can be referred to as colours, depending on how it is produced. The most common production process is via steam methane reforming (SMR) with natural gas as feedstock, known as 'grey H_2'. Further, if carbon capture and storage (CCS) is added, it is referred to as 'blue H_2'. There is a possibility to replace natural gas with biomethane as feedstock in the SMR process, which is referred to as 'beige H_2' in this study, and with CCS it can be called 'orange H_2'. Another production technology is through water-electrolysis, which is referred to as 'green H_2'.

A life cycle assessment (LCA) based methodology was performed, in which the greenhouse gas emissions from "well-to-wheel" were investigated for each H_2 colour as fuel for heavy truck transport. The result shows that orange H_2 could provide negative emissions, due to its service of capture CO_2. Beige and green H_2 are close to being climate neutral, while grey and blue H_2 contribute with higher emissions. When H_2 is implemented in the heavy transport sector, a mix of different H_2 colours is most likely necessary, depending on the political and geographical context.

Populärvetenskaplig sammanfattning

Vätgas är ett möjligt bränsle i en framtida transportsektor, och kan bidra till att nå Sveriges nationella miljömål om nettonollutsläpp till 2045. Tunga fordon och långdistanstransport har stora potentialer att använda vätgas som bränsle genom en bränslecell, där elektriska batterifordon inte är optimala. Bränslecellsfordon resulterar endast i vatten som direkta utsläpp vilket gör vätgas fördelaktigt som bränsle i en framtida koldioxidfri transportsektor.

Genom en livscykelanalysbaserad metod har det påvisats att klimatpåverkan från vätgas varierar till stor del beroende på produktionsprocess. Idag är den vanligaste produktionsprocessen för vätgas genom ångmetanreformering med naturgas som råvara, vilket kallas grå vätgas och bidrar enligt studien med 2% lägre klimatgasutsläpp än för en diesellastbil. För att minska utsläppen kan koldioxidavskiljning och lagring (CCS) implementeras där koldioxid (CO_2) fångas in och lagras under havsbotten. Vätgas från ångmetanreformering med CCS kallas blå vätgas, och släpper enligt studien ut 36% mindre växthusgaser än en diesellastbil. Om naturgas byts ut mot biometan som råvara fås beige vätgas, vilket bidrar till att minska utsläppen med 75%. Det är även möjligt att implementera CCS teknik intill anläggningen för ångemetanreformering med biometan, vilket kallas orange vätgas och kan bidra med negativa klimatgasutsläpp. Jämförs en bränsecellsdriven lastbil från orange vätgas med en dieseldriven lastbil kan en utsläppsminskning på 110% ses. Om vätgas istället produceras genom vattenelektrolys med förnybar elektricitet kallas det grön vätgas, och bidrar till nära nettonollutsläpp samt 95% utsläppsminskning jämfört med diesel.

Studien visar på betydelsen av att undersöka hela livscykeln av ett bränsle, eftersom de direkta utsläppen från vätgas som bränsle endast är vatten, medan produktionsprocessen påverkar utsläppen av klimatgaser. Både grå och blå vätgas produceras av fossila bränslen, vilket i Sverige troligtvis endast kommer användas som en kort övergång till hållbara produktionsprocesser. Beige och orange vätgas kan i dagsläget endast produceras småskaligt, och är begränsat av mängden avfall som biogas produceras av. Om negativa utsläpp däremot skulle kunna vara en tjänst som går att sälja i framtiden skulle orange vätgas troligtvis kunna växa genom ökad ekonomisk lönsamhet. Grön vätgas kommer troligtvis öka mest i Sverige, förutsatt fortsatt låga elpriser och hög tillgänglighet på vind-, vatten- eller solkraft.

Hur vätgas produceras kan även anpassas till vilka resurser och politiskt styre som respektive område har. I regioner med låga elpriser och hög tillgänglighet på förnybar el är grön vätgas ett bra val. Om elpriserna istället är höga kan någon av

de andra vätgasfärgerna vara bättre. I områden med hög biogasproduktion kan beige och orange vätgas vara ett bra alternativ, och där CCS teknik är högt politiskt accepterat kan blå och orange vätgas istället vara en bra kombination. Grå vätgas kommer troligtvis inte öka mycket mer eftersom utsläppen av växthusgaser är höga och fossila bränslen används.

Vätgas- och eldrivna fordon kan i en framtida transportsektor komplettera varandra då vätgas har stora potentialer att användas i tung fordonstrafik medan eldrivna fordon kan användas för personbilar och lättare fordon. I den här studien har olika framtidsscenarier utformats där vätgas successivt ersätter diesel som bränsle för tunga lastbilar. Vidare har den globala temperaturförändringen använts som en indikator för klimatpåverkan. Resultaten visar att diesel tillsammans med grå vätgas bidrar till högst klimatpåverkan i form av global temperaturhöjning, medan orange- och grön vätgas bidrar till lägst temperaturförändring. Även om vätgas kan vara ett stort bidrag till att minska utsläppen i en framtida transportsektor krävs även fler förnybara drivmedel för att nå målet om nettonollutsläpp till 2045.

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After six years of university studies, including one exchange year in Spain, it is now time for next chapter!

Madeleine Stolpe
June 2021

Abbreviations

H_2	Hydrogen
CO	Carbon monoxide
O_2	Oxygen
CO_2	Carbon dioxide
CH_4	Methane
N_2O	Nitrous oxide
GHG	Greenhouse gases
SMR	Steam methane reforming
WGS	Water gas shift
PSA	Pressure swing adsorption
CCS	Carbon capture and storage
TRL	Technology readiness level
AEL	Alkaline electrolysis
PEM	Proton exchange membrane
AEMEL	Anion exchange membrane electrolysis
SOEL	Solid oxide electrolysis
LCA	Life cycle assessment
GWP	Global warming potential
AGTP	Absolute global temperature change potential
WTW	Well-to-wheel
WTT	Well-to-tank
HHV	Higher heating value
LHV	Lower heating value
FCEV	Fuel cell electric vehicles
BEV	Battery electric vehicles

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1. Introduction

The transition of the energy system will require a large amount of renewable energy sources to meet the target of staying well below 2 °C temperature increase from the Paris Agreement. In a future decarbonized energy system, hydrogen (H_2) has been proposed to play a major role as it can be used to replace fossil fuels in the industry, generate electricity for the power grid and be used as a fuel in the transportation sector (Fuel Cells and Hydrogen Joint Undertaking 2019).

The Swedish transportation sector covers one third of the total greenhouse gas (GHG) emissions, where domestic road transport counts for 90% of its total emissions (Trafikverket 2020b). Hydrogen can play a major role in reducing the environmental and climate impacts of the transportation sector. Using H_2 as a fuel in vehicles only results in pure steam emissions from the exhaust pipe. The most common technology for H_2 vehicles is by using a fuel cell in combination with a battery. A fuel cell is an energy converter that can be used to convert the chemical energy of H_2 into electricity, with water and heat as by-products. The efficiency of a fuel cell electric vehicle (FCEV) is around twice as high as for a conventional combustion engine, which can make up for the energy required for the H_2 production process (Vätgas Sverige 2019). Due to the high energy density of H_2, FCEVs are beneficial for long distance and heavy transportations. Battery electric vehicles (BEV) require larger and heavier batteries than FCEVs and are therefore well suited for smaller passenger cars while FCEVs are beneficial for larger passenger cars and heavy trucks. In a future transportation sector, FCEV and BEV will likely complement each other (Fuel Cells and Hydrogen Joint Undertaking [FCH JU] 2019).

However, to meet the transition of a decarbonized transportation sector, the H_2 production processes must become climate neutral. Today, the most common feedstock for H_2 production is from fossil fuels, which contributes to annual emissions of 70 – 100 million tonnes CO_2 within the European Union (EU) (European Commission 2020). The aim of this thesis is to understand how and at what rate H_2 could effectively contribute to a decarbonized transportation sector. This is done by assessing the climate impact of the life cycle of H_2 with different production processes. Further, the temperature response of implementing H_2 as a fuel in heavy truck transportation is assessed, using a time-dependent life cycle assessment (LCA) based methodology. The aim of the thesis will be reached by answering the following questions:

- What climate impact can hydrogen cause when using natural gas as feedstock?
- What climate impact can hydrogen cause when using biomethane as feedstock?
- How much could adding carbon capture and storage help mitigate climate impact from the hydrogen life cycle?
- What climate impact can hydrogen cause when using water-electrolysis as production process?
- What could the technology deployment of different hydrogen production processes look like in a future decarbonized heavy road transport sector?
- What climate impact can future heavy road transport cause- if hydrogen displaces diesel as fuel?

2. Background

In this section, the different H_2 production processes are described, beginning with steam methane reforming (SMR) and the possible feedstocks, followed by carbon capture and storage (CCS) and finishing with water-electrolysis production technologies. After that, the LCA methodology is described, including climate impact metrics, and lastly, the goal and scope of the study is defined.

2.1. Hydrogen production processes

There are a variety of production processes today, often referred to as different colours depending on the production technology (IEA 2019). Currently, the most common technology for large-scale production is SMR, mainly with natural gas as feedstock (Nikolaidis & Poullikkas 2017). This production process is referred to as 'grey H_2' and due to the fossil feedstock, it results in high emissions of greenhouse gases (GHG). However, the emissions of carbon dioxide (CO_2) could reduce by implementing CCS technology in connection with the SMR plant. Hydrogen production via SMR with CCS is referred to as 'blue H_2'. Although grey H_2 is the dominant production process on the market, several blue H_2 production plants are in operation (IEA 2019).

Another upcoming production technology is through water-electrolysis from renewable electricity, called 'green H_2' (Velazquez Abad & Dodds 2017). Although this technology could contribute with fewer emissions than grey and blue H_2, green H_2 faces barriers on the market due to the expensive electrolytic technologies. Currently, green H_2 costs 2–3 times more than blue H_2 (IRENA 2020).

However, if natural gas could be replaced with biogas in the SMR process, it could result in net-zero emissions of CO_2. Biogas has the advantage of generally being considered carbon neutral as the CO_2 that is emitted from the process and combustion has been taken up by the biomass via photosynthesis during plant growth (Antonini et al. 2020). In addition, if CCS technology is implemented in the SMR plant, it could potentially result in negative emissions of CO_2 (Antonini et al. 2020). In this thesis, H_2 production from biogas via SMR is referred to as 'beige H_2', and with CCS implementation it is called 'orange H_2'.

2.1.1. Steam methane reforming

In the SMR process, methane (CH_4) and water (H_2O) in the form of steam are used to produce syngas, which is further converted into H_2 by a water-gas shift (WGS) reaction. The conversion is performed in two steps, expressed in equation 1 and 2 (Timmerberg et al. 2020).

$$CH_4 + H_2O \rightarrow CO + 3H_2 \qquad \Delta H = 206.2 \text{ kJ/mol} \qquad (1)$$

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad \Delta H = -41.2 \text{ kJ/mol} \qquad (2)$$

The energy conversion efficiency of the SMR plant is typically 74-85% and can operate in both large- and small-scale systems (Nikolaidis & Poullikkas 2017). Before entering the reformer, the feedstock is desulfurized to avoid contaminations. The desulfurized natural gas enters the reformer where CH_4 and H_2O react to produce a H_2 rich syngas with carbon monoxide (CO) as by-product (Soltani et al. 2014), see equation 1. This reaction is highly endothermic and requires high temperatures at 700–1000 °C which is generated by an external furnace (Nikolaidis & Poullikkas 2017). The furnace is fuelled by additional natural gas, which covers 30–40% of the total amount of the natural gas consumed. The additional 60–70% of the natural gas is used as feedstock to produce H_2 (IEA 2020a).

To increase the yield of H_2, the by-product CO undergoes a WGS reaction (equation 2). Carbon monoxide enters the WGS unit and together with additional steam it produces H_2 and CO_2. The WGS reaction is exothermic and produces a small amount of waste heat (Navas-Anguita et al. 2021). The produced H_2 undergoes a purification step, commonly through pressure swing absorption (PSA) (Timmerberg et al. 2020). Through separation with PSA, H_2 can reach up to 99.999% of purification (Nikolaidis & Poullikkas 2017). A simplified illustration of the SMR process is demonstrated in figure 1.

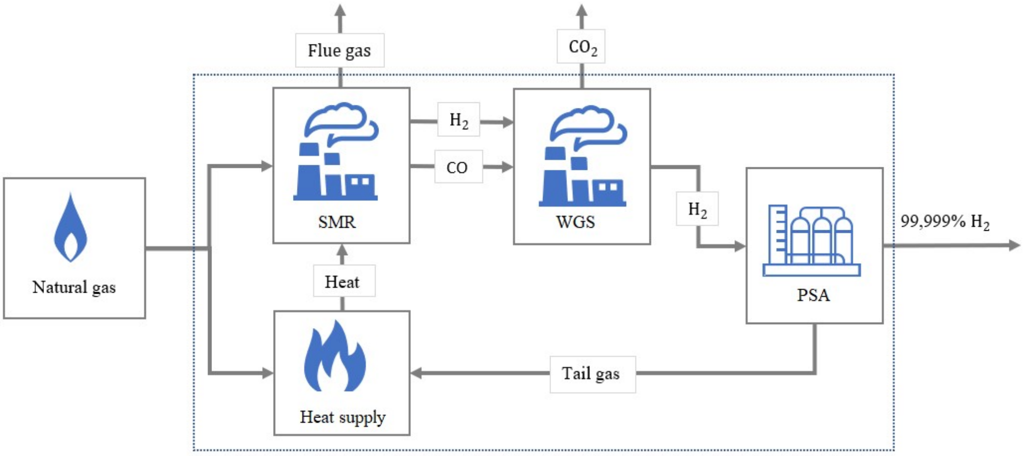

Figure 1. Illustration of the steam methane reforming process with the units of SMR, WGS, PSA and the external furnace.

Feedstock for the SMR process

Currently, natural gas is the most common feedstock for the SMR process (IEAGHG 2017). Natural gas is a CH_4 rich energy gas and can be used as a gas or a liquid. Since Sweden does not have domestic production, the country is dependent on natural gas imports from Denmark to the west coast pipeline network, and imports of liquified natural gas (LNG) to the gas grid of Stockholm (Energimyndigheten 2020). The CH_4 composition of LNG depends on the geographical location and the CH_4 content can vary from 87–99%. Norwegian produced LNG contains approximately 92% CH_4 (Kuczyński et al. 2020), and can be exported by ship to Sweden via LNG terminals in Lysekil and Nynäshamn (Boëthius 2020).

Biomethane could be a fossil free alternative as feedstock for conventional H_2 production via SMR. It has similar compositions as natural gas with additional benefits, as it is a renewable resource (Braga et al. 2013). Biogas is produced from organic feedstocks processed by anaerobic digestion. It mainly contains CH_4 and CO_2, with a CH_4 quality of 45–75%. To enable its use as vehicle fuel, biogas is upgraded by removing most of the CO_2 content. The near-pure CH_4 gas is known as biomethane and can replace natural gas in the SMR process (IEA 2020b).

Carbon capture and storage

The SMR process has two streams of emissions, approximately 60% of the CO_2 is emitted from the feedstock during the reforming and shift reactions, referred to as pre-combustion. The remaining 40% is emitted from the flue gas during heat generation in the external furnace, known as post-combustion. Thus, the emissions from the SMR plant can be reduced significantly by implementing a CCS unit in connection with the emission streams (Antonini et al. 2020). The capture rate of CO_2 is between 54–90% depending on the technology and location of the CCS unit (Timmerberg et al. 2020). The capture cost of the CCS plant is dependent on the concentration of CO_2. The pre-combustion stream is more concentrated and costs around 50 USD/tCO_2, while the post-combustion stream is more diluted. The costs increase to around 80 USD/t if additional CO_2 is captured from the post-combustion stream (IEA 2020a).

Currently, there is a wide variety of the maturity of CCS technologies. The International Energy Agency (2020a) performed an evaluation of different CCS technologies. It was based on a technology readiness level (TRL) scale, which measures the maturity of a technology, based on the development from the laboratory to the market. The evaluation shows the most mature CO_2 capture technology to be amine based chemical absorption and the most mature CO_2 storage technology to be enhanced oil recovery, followed by saline formations. However, the storage technology depends on the geological conditions (SGU 2020).

Currently, there are CO_2 storage sites in various places in North America and China. Other countries that have CCS projects in commercial operation are Brazil, Australia and Qatar. In Europe, the only commercial storage site is in Norway (SCCS 2021).

Due to the geological formations of saline aquifers in the Norwegian North Sea, Norway has experience with CCS since 1996 (Ringrose 2018). The Norwegian Government's full-scale CCS project is called Northern Lights (Riis 2018), and is used as a reference for this study. Before CO_2 storage, the gas is compressed and liquefied, to be transported from the capture site to an onshore terminal on the west coast of Norway. From the terminal, liquefied CO_2 is transported through pipelines to a deep reservoir in the Norwegian North Sea, located 2600 meters below seabed, where CO_2 can be permanently stored (Northern Lights CCS 2020). In Sweden, an ongoing project named CinfraCap is aiming to reach a mutual solution for logistics and infrastructure of liquified CO_2. CinfraCap completes many ongoing research and demonstration projects and will connect domestic CO_2 capture projects in Sweden with a buffer storage at Gothenburg port. The permanent storage follows the Northern Lights project in Norway (Göteborgs hamn 2021).

2.1.2. Electrolysis based on renewable energy

Another H_2 production technology is via water-electrolysis from renewable electricity. The electrolytic cell has a positively charged anode and a negatively charged cathode in water, which works as a conductive medium. When an electric current is added, the positively charged hydrogen ions are attracted to the cathode and the negatively charged oxygen ions to the anode. Consequently, the process splits water into H_2 and oxygen (O_2) (Velazquez Abad & Dodds 2017). The stoichiometric relation is expressed in equation 3.

$$\mathrm{H_2O} + \mathrm{energy} \rightarrow \mathrm{H_2} + \frac{1}{2}\mathrm{O_2} \tag{3}$$

Hydrogen production from water-electrolysis, with electricity from renewable sources such as wind or solar power is in line with reaching a net-zero carbon energy system. However, H_2 production from electrolysis only accounts for 5% of the global H_2 production today, which is mainly due to the expensive production process (IRENA 2020).

Currently, the most implemented electrolytic technology is alkaline electrolysis (AEL). Proton exchange membrane (PEM) electrolysis is another upcoming technology but not yet as established as AEL (FCH JU 2019). The capital costs differ between the two technologies as PEM requires expensive material like noble metals, however it has a more compact design. Also, the response time is faster with

PEM. The advantages of AEL are the lower costs and the simpler design with cheaper materials. However, for future electrolytic processes, there are possibilities to combine the two technologies to an anion exchange membrane electrolysis (AEMEL). Although the AEMEL technology would achieve lower costs and higher stability, it is not yet largely commercialized. Another electrolytic technology that is developing is solid oxide electrolysis (SOEL), which could contribute to higher efficiencies. Also, this technology allows reverse operations, which could provide services for balancing the grid by converting H_2 back to electricity. Although the SOEL electrolyte has high efficiency and smart solutions for grid balancing, it requires high temperatures which currently leads to low stability and high costs (Formann et al. 2020).

2.2. LCA methodology and climate impact

Life cycle assessment is a method that can be used to assess the environmental impact of a product or process, including impacts throughout the entire life cycle. There are four main steps considered when performing an LCA; goal and scope, life cycle inventory, life cycle impact assessment and interpretation of results (Muralikrishna & Manickam 2017). The environmental impact of a product or process can be measured in various ways including global warming, acidification, water use and biodiversity (Guinée et al. 2011). When performing an LCA, a functional unit is used to compare different systems that achieve the same purpose.

The most common greenhouse gases emitted to the atmosphere by human activities are CO_2, CH_4 and N_2O. When combusting fossil fuels, solid waste or other biological materials, CO_2 is emitted to the atmosphere. In a balanced biogenic carbon cycle, the same amount of CO_2 that is emitted would be absorbed by the plants. Methane is a GHG that is emitted when producing and distributing coal, natural gas and oil. Also, CH_4 is emitted during agricultural processes and from the organic waste in municipal solid waste. The third most common GHG is N_2O which is emitted when combusting fossil fuels and solid waste as well from agricultural production and processes (US EPA 2015).

The climate impacts from GHG emissions can be compared using different climate metrics. The global warming potential (GWP) is one way of comparing the climate effects of GHG emissions (IPCC 2013). By using the GWP over a 100 year time horizon (GWP_{100}), the CO_2-equivalents can be calculated. In the 5th IPCC Assessment Report (2013), the GWP_{100} was determined to 1 for fossil CO_2, 0 for biogenic CO_2, 30 for fossil CH_4, 28 for biogenic CH_4 and 265 for N_2O. Another climate metric that can be used to compare climate impacts from different emissions is the absolute global temperature change potential (AGTP). AGTP is defined as the surface temperature for a specific point in time, due to an emission impulse expressed in K/kg (Fuglestvedt et al. 2010).

2.3. Goal and scope

The goal of the LCA study in this thesis project was to find the life cycle GHG emissions for grey, blue, beige, orange and green H_2. Further, the temperature response of the heavy truck transportation when displacing diesel with H_2 was found by assessing future scenarios representing different deployment rates of H_2 colours. The only considered environmental impact category was climate impact, which was assessed using the GWP and AGTP. Since H_2 was used as fuel in heavy truck transport, the emissions were compared for transporting one tonne over one kilometer, and the functional unit was set to *tonne-km.*

To perform the study, some assumptions were made. The production plant was assumed to be placed in Uppsala, where the total domestic production of H_2 was produced. The amount of produced H_2 was assumed to cover the entire domestic transportation of heavy diesel trucks in Sweden. Natural gas based H_2 was assumed to be produced from Norwegian LNG. The assumption was based on the Stockholm gas grid, which is fed by LNG through the port of Nynäshamn (Energimyndigheten 2017). Biomethane based H_2 was assumed to be produced in close connection to the H_2 production plant. The organic waste for biogas production was assumed to come from sewage sludge and municipal solid waste, which set limitations for biomethane based H_2 production. Water-electrolysis based H_2 was assumed to be produced by electricity from wind power in Sweden. From this, the feedstocks of natural gas and wind powered electricity were assumed to be unlimited and meet the H_2 demand to cover the diesel share for heavy truck transportation. Biogas on the other hand, was assumed to be limited by the availability of organic waste. Regardless H_2 colour, the production plant was assumed to operate for 30 years, which set the time horizon of the future scenarios. The deployment of the different H_2 colours in the future scenarios was assumed to be based on production costs as well as feedstock availability for H_2 production. The number of heavy trucks and the fuel consumption in the future scenarios were assumed to remain constant for the study time of 30 years.

The system boundaries include the GHG emissions of CO_2, CH_4 and N_2O, from well-to-wheel (WTW). Emissions from construction and maintenance of the production plants were excluded, and so were the people that contribute to operations. Collection and transport of raw material to the biogas plant were not included. The process tree for the H_2 life cycle is shown in figure 2.

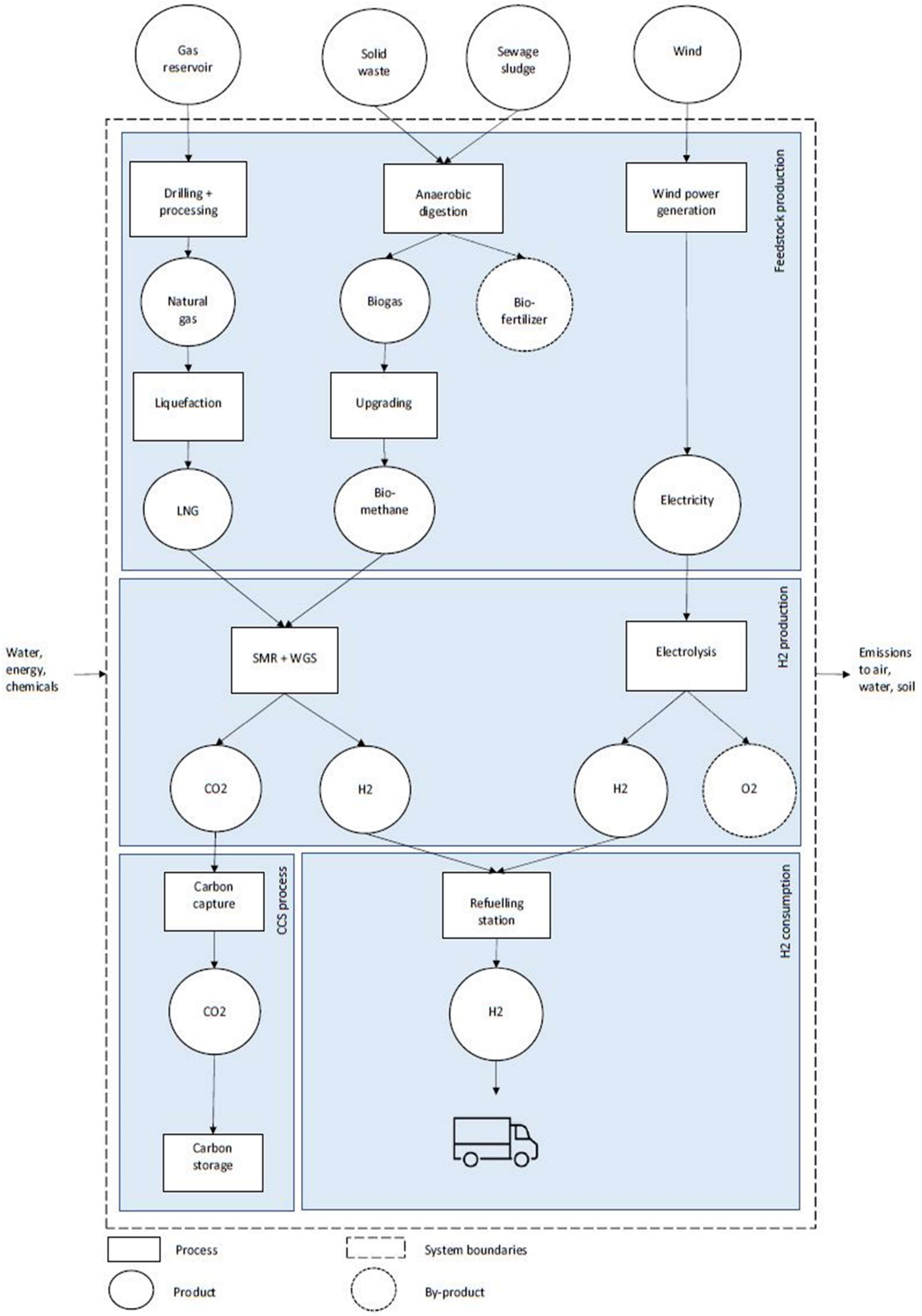

Figure 2. The process tree of the studied system illustrates the scope and limitations of the system as well as the product flow and process steps.

3. System model

In this section, the H_2 models are described, beginning with the colour definitions, followed by H_2 implementation in a future transportation sector. To implement H_2 as a fuel for heavy trucks, future scenarios were developed, in which different mixes of H_2 colours are implemented at different deployment rates. A market analysis is carried out followed by a definition of the different future scenarios for heavy truck transport.

3.1. Hydrogen colours

The H_2 colours are defined by different production processes. In this section, systems are described and flow diagrams are demonstrated for each H_2 colour. Assumptions and data of geographical locations, fuel consumption and electricity sources are explained for each process.

3.1.1. Grey H_2

Hydrogen is produced from an SMR plant in Uppsala, using natural gas as feedstock. Natural gas is assumed to be produced in Norway and compressed and shipped from Risavika port to Nynäshman, as liquefied natural gas (LNG). The ships are assumed to be fuelled with bunker oil. From Nynäshamn, LNG is transported in trucks to Uppsala, fuelled with diesel mixed with 5% RME. As a simplification of the system, no sub-storage of LNG is considered.

The energy conversion efficiency of the SMR plant is 78%, and the electricity consumption is 2.6 kWh/kg H_2 (Valente et al. 2020). The emission factor of the used electricity is 338.52 g CO_2-eq/kWh, which represents the Nordic residual mix for 2019. The residual mix is the electricity that is bought if no specific electricity source or origin-marking is chosen (Energimarknadsinspektionen [Ei] 2020), which is assumed for the electricity consumption in the SMR plant. When H_2 is produced and purified, it is distributed to a fuel station in close connection to the SMR plant. The process is demonstrated in figure 3.

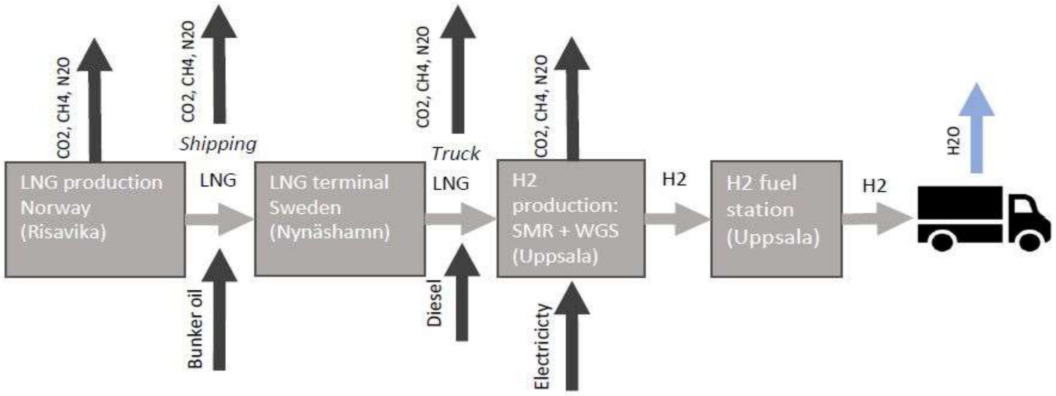

Figure 3. Flow chart of grey H_2. Horizontal arrows show the flow of products while vertical arrows show exchanges with the environment and upstream systems.

3.1.2. Blue H_2

Blue H_2 follows the same process steps as grey H_2, but with CCS added in connection to the SMR plant. The CCS unit is placed in connection to the pre-combustion stream, and covers 60% of the total CO_2 emissions (Antonini et al. 2020), with a capture efficiency of 90% (Skagestad et al. 2017). The total energy consumption of the CCS unit is 0.279 kWh/kg CO_2 (IEAGHG 2010), and is assumed to be covered by electricity from the Nordic residual mix. When the CO_2 is captured, it is compressed and liquified. Further, CO_2 is transported in trucks from Uppsala to a buffer storage at Gothenburg port, followed by shipping from Gothenburg to an onshore CO_2 terminal outside Bergen, Norway. From the terminal, the liquefied CO_2 is transported through pipelines to a permanent storage, in deep saline aquifers, 2600 meters below the seabed of the Norwegian North Sea. The assumptions of the CO_2 transportation and storage process are based on the CinfraCap and Northern Lights project. The full process of blue H_2 is demonstrated in figure 4.

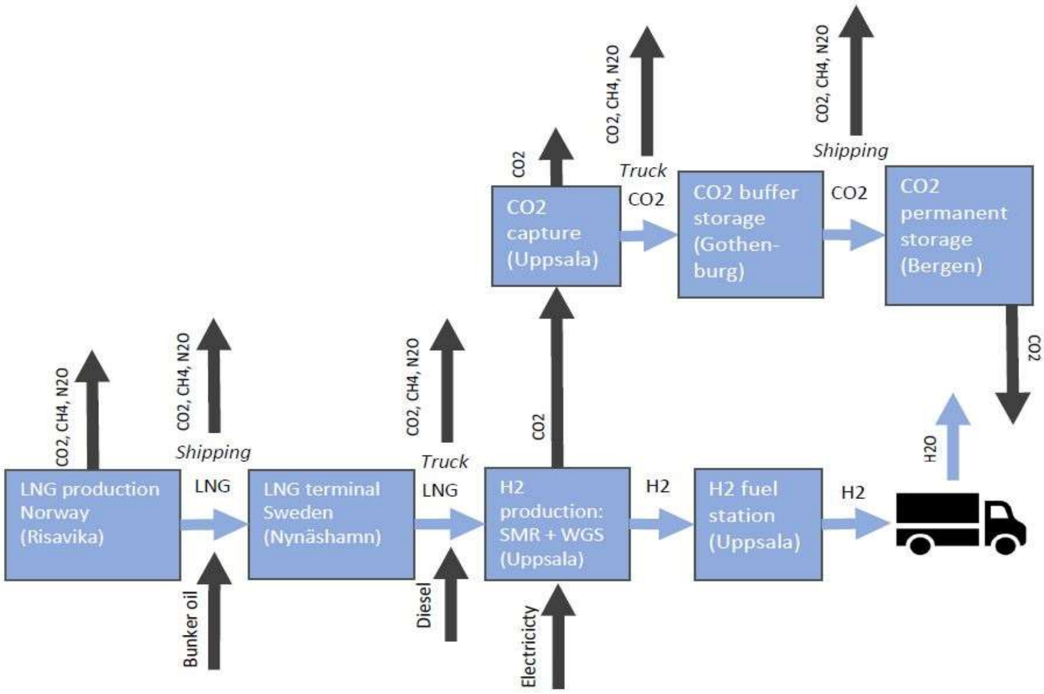

Figure 4. Flow chart of blue H_2. Horizontal arrows show the flow of products while vertical arrows show exchanges with the environment and upstream systems.

3.1.3. Beige H_2

Beige H_2 follows the same process steps as grey H_2, but natural gas is replaced with biomethane, which is upgraded biogas that is derived from anaerobic reactors treating sewage sludge and organic fraction of municipal solid waste. No energy crops such as maize or beets are used in this study. The production rate is 0.62 m^3 bio-CH_4/m^3 biogas (Florio et al. 2019) and the CH_4 leakage from the upgrading process is assumed to be 1.4% (Holmgren et al. 2015). The CO_2 emissions from the biogas production and upgrading is 0.58 kg CO_2/m^3 (Florio et al. 2019). The electricity consumption is 0.33 kWh/m^3 biogas which was calculated as mean value from Zhang et al. (2020) and Florio et al. (2019). Furthermore, the SMR plant and the H_2 fuel station are assumed to be in close connection to the biogas upgrading plant. No transportation between biomethane production, H_2 production and fuel station is assumed. Flow chart of beige H_2 is shown in figure 5.

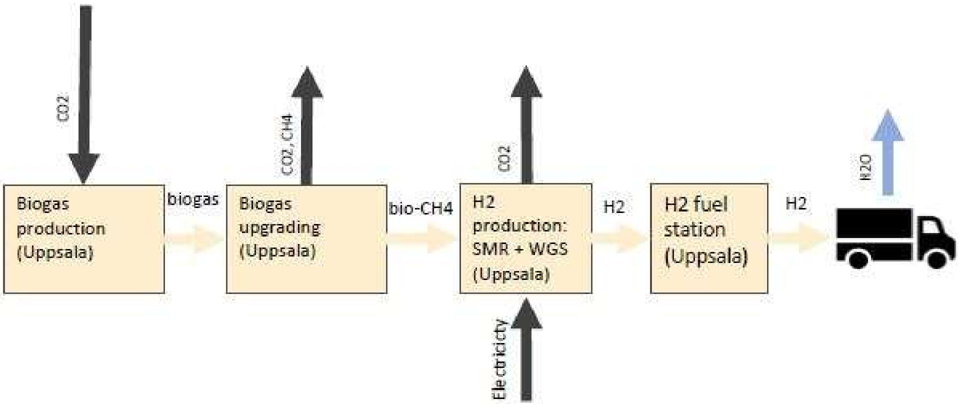

Figure 5. Flow chart of beige H_2. Horizontal arrows show the flow of products while vertical arrows show exchanges with the environment and upstream systems.

3.1.4. Orange H_2

Hydrogen is produced through the same process as beige H_2, but with CCS added. Same feedstock is used as for beige H_2, and the CCS properties are the same as in blue H_2. Flow chart is presented in figure 6.

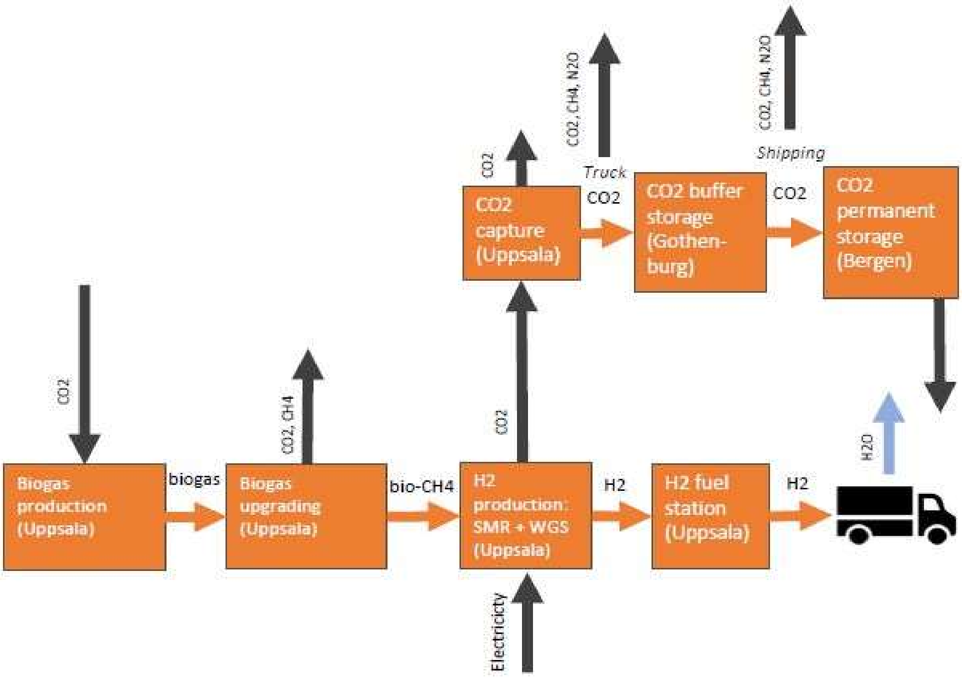

Figure 6. Flow chart of orange H_2. Horizontal arrows show the flow of products while vertical arrows show exchanges with the environment and upstream systems.

3.1.5. Green H_2

Hydrogen is produced from renewable electricity via water-electrolysis. The electrolytic unit is located in connection to a H_2 fuel station in Uppsala, Sweden. The most established water-electrolysis technology is alkaline electrolysis (FCH JU 2019), which is the chosen electrolytic technology for this study. The required electricity for the electrolysis process is 54.18 kWh/kg H_2 (Valente et al. 2020). Due to the high electricity demand, green H_2 is highly dependent on the electricity source. The electrolytic plant is connected by the grid and for this study, the electricity is assumed to be bought from wind power specifically. The emission factor of wind power is 15 g/kWh (Gode et al. 2011). The flow chart is shown in figure 7.

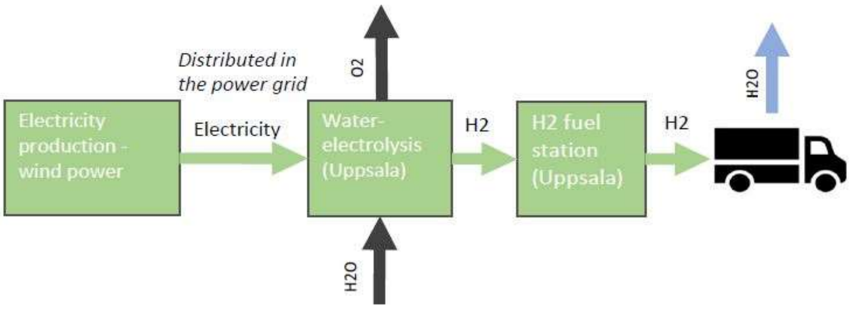

Figure 7. Flow chart of green H_2. Horizontal arrows show the flows of H_2 while vertical arrows are emissions and resource inputs for each process.

3.2. Hydrogen in future heavy truck transportation

The major fuel for heavy truck transportation in Sweden is diesel, which covers 92% of the total fuel demand (Trafikverket 2020a). Future scenarios are defined with different deployment rates of H_2 when displacing diesel as a fuel for heavy truck transportation. The future scenarios are based on a market analysis and a hydrogen roadmap for Europe, prepared by Fuel Cells and Hydrogen Joint Undertaken (FCH JU), where a proposal of H_2 implementation in the EU through different future scenarios was presented. FCH JU (2019) claims that an ambitious target is required to achieve the limit of staying well below 2 °C temperature increase, proposed by the Paris Agreement. Within the entire energy sector, H_2 could provide up to 6% of the total energy demand in the EU by 2030, and 24% by 2050. Within the transportation sector in the EU, H_2 could provide 70 TWh by 2030 and 675 TWh by 2050.

3.2.1. Market analysis

Today, the production cost in Europe of H_2 via SMR process is between 1.7 USD/kg H_2 for production without CCS (grey H_2) and 2.4 USD/kg H_2 for production with

CCS (blue H_2) (IEA 2019). Beige and orange H_2 are unlikely to be feasible in large-scale plants due to limitations in biogas availability, which may increase its production costs considerably. However, orange H_2 offers the possibility to generate negative emissions, therefore additional payments for this service are expected to improve the feasibility of this process in the future. In the Climate Political Roadmap Report (sv. Klimatpolitiska vägvalsutredningen 2020), a public report from the Swedish Government, it was discussed how to reach negative emissions by 2045. The Swedish Government proposed an auction system as a tool to reach the climate target. This tool would encourage bio-CCS projects by supporting them with reversed auctions that could compensate for the investment costs. If this would be implemented, orange H_2 could compete with grey and blue H_2. However, beige and orange H_2 would be limited by the availability of biogas.

Regarding green H_2, the production costs in 2020 varied between 2.1-5.1 USD/kg H_2, depending on CAPEX and electricity prices. After 2025, green H_2 is expected to be competitive with grey and blue H_2 in countries with cheap electricity and good conditions for wind or solar power, due to new developments and cheaper production costs (IRENA 2020). This will make green H_2 the dominant colour due to its multiple benefits from using renewable energy, lower carbon footprint and its high political acceptance in Sweden. According to the market analysis by FCH JU (2019), H_2 production from electrolysis could account for 20-60% in 2030, and after that, the mix of production technologies is dependent on the economic situation and cost development.

Further, Navas-Anguita et. al. (2020) assessed the investment costs of H_2 in Spanish road transportation. The study shows that for the short-term deployment of FCEV, grey H_2 is most likely to be dominant. However, for the mid- and long-term, green H_2 can be the key production process. The investment costs of different H_2 production processes are shown in table 1.

Table 1. Investment costs of different H_2 production technologies (Navas-Anguita et al. 2020)

	2016 [€/GJ]	**2030** [€/GJ]	**2050** [€/GJ]
SMR with natural gas	8.75	7.33	7.33
SMR+CCS with natural gas	14.50	11.10	9.44
Electrolysis	36.76	15.86	6.10

3.2.2. Future scenarios

The future scenarios illustrate the deployment rates of different H_2 colours when displacing diesel as fuel for heavy trucks in Sweden and are illustrated in figure 8. In the reference scenario, the diesel share for heavy truck transport remains constant over the next 30 years. This scenario represents the heavy truck transportation if no

H_2 is implemented, and the fuel consumption of conventional diesel trucks remains the same.

Scenario 1 represents an SMR dominant scenario with natural gas as feedstock, consisting of only grey and blue H_2. This scenario assumes low natural gas prices and high electricity costs. Further, the deployment of electrolytic technologies is low. Grey H_2, which is the cheapest H_2 today, only works as a bridge solution before introducing blue H_2. For scenario 1 it is assumed that the political acceptance of CCS technologies increases with time, which motivates further implementation of blue H_2.

Scenario 2 represents an SMR dominant scenario, where natural gas is replaced with biomethane as beige and orange H_2 are introduced. However, biomethane is limited by biogas production, which in turn is limited by the municipal solid waste. It is assumed that biogas will continue to be produced from co-digestion and waste-water treatment plants throughout the next 30 years, which limits the share of beige and orange H_2.

Scenario 3 represents a mix of all H_2 colours, with a rapid increase of green H_2 after 2030. This scenario assumes increased technological developments and reduced investment costs of electrolytic processes, while electricity prices are low and renewable electricity production is high.

Two extreme scenarios are included, where extreme scenario 1 shows the H_2 implementation of only grey H_2, assuming low natural gas prices and low acceptance of CCS. Extreme scenario 2 contains only orange H_2 as displacement for diesel, which assumes increased biogas production and high political acceptance of CCS.

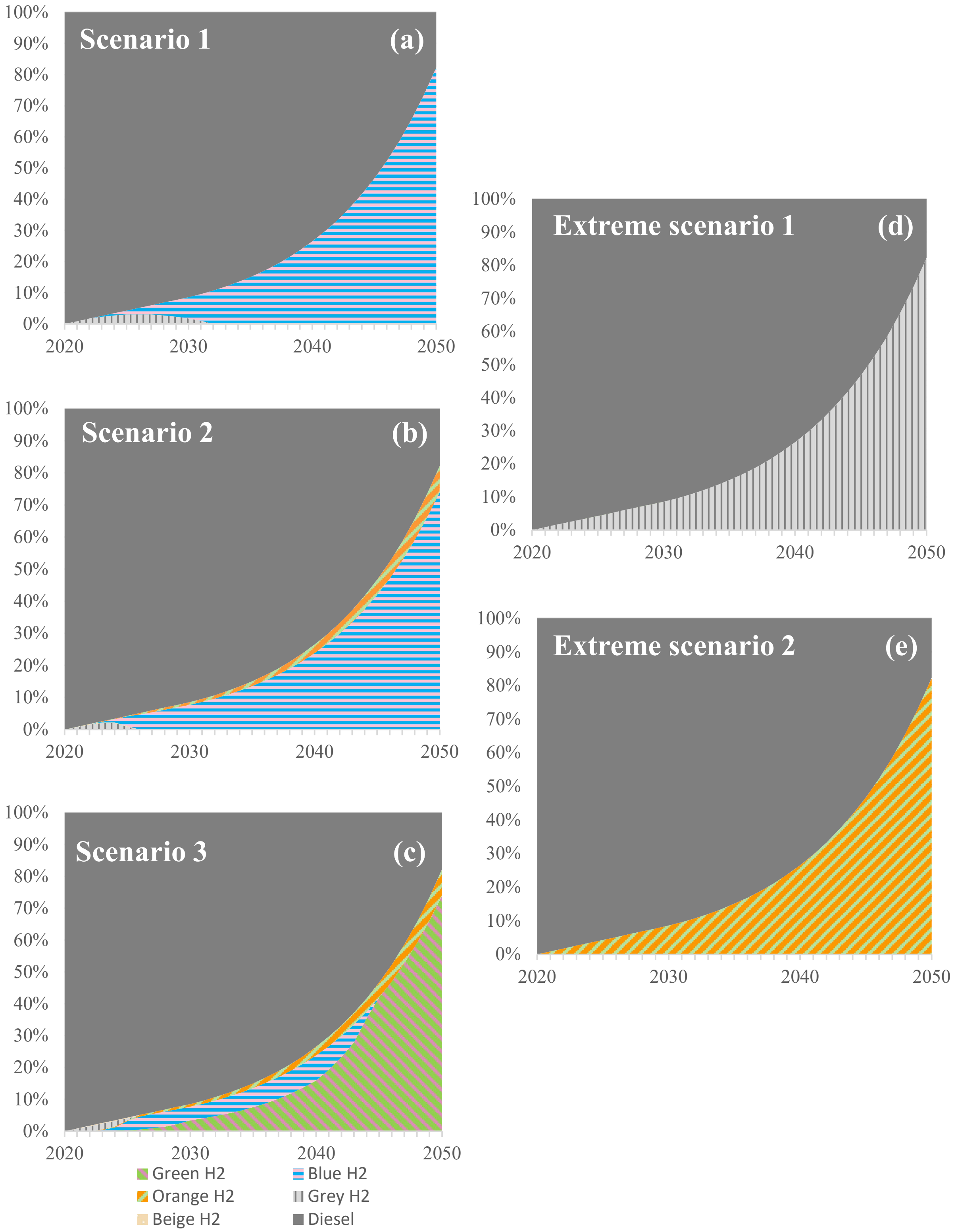

Figure 8. The share of diesel, grey, blue, beige, orange and green H_2 in a future heavy truck transportation. Scenario 1 (a) is SMR dominant with natural gas, scenario 2 (b) is SMR dominant with natural gas and biomethane, scenario 3 (c) is electrolysis dominant with a mix of all H_2 colours. Extreme scenario 1 (d) illustrates diesel displacement with only grey H_2 while extreme scenario 2 (e) represents diesel displacement with orange H_2.

4. Methodology

In this section, the calculation methodology is described step by step. First, mass and energy balances were calculated for the SMR and electrolytic processes. Second, the WTW emission data was collected, and the inventory was calculated for each process. Third, time-dependent calculations were performed from the future scenarios and finally, a sensitivity analysis was carried out.

4.1. Mass- and energy balance

Mass balances ($x_{H2O}, x_{CO}, x_{H_2}, x_{CO_2}$) were calculated for the SMR and WGS processes using the stoichiometric approach and the molecular masses of m_{CH_4}=16.043 u; m_{H2O}=18.015 u; m_{CO}=28.01 u; m_{H_2}=2.016 u. Calculations of mass balances followed equations in table 2, where 1 kg CH_4 was used (x_{CH_4}).

Table 2. Equations for the mass balance of SMR and WGS processes.

SMR reaction	**WGS reaction**
$CH_4 + H_2O \rightarrow CO + 3H_2$	$CO + H_2O \rightarrow CO_2 + H_2$
$x_{H2O} = x_{CH_4} \cdot \frac{m_{H2O}}{m_{CH_4}}$	$x_{CO} = x_{CH_4} \cdot \frac{m_{CO}}{m_{CH_4}}$
$x_{CO} = x_{CH_4} \cdot \frac{m_{CO}}{m_{CH_4}}$	$x_{H2O} = x_{CO} \cdot \frac{m_{H2O}}{m_{CO}}$
$x_{3H_2} = x_{CH_4} \cdot \frac{m_{3H_2}}{m_{CH_4}}$	$x_{CO_2} = x_{CO} \cdot \frac{m_{CO_2}}{m_{CO}}$
	$x_{H_2} = x_{CO} \cdot \frac{m_{H_2}}{m_{CO}}$

Energy balances were calculated using lower heating values of LHV_{CH_4}=50 MJ/kg, LHV_{H_2}=119.9 MJ/kg (Nikolaidis & Poullikkas 2017) and LHV_{CO}=10.16 MJ/kg (Engineering ToolBox 2005). The SMR process is endothermic and requires a heat supply, whereas the WGS process is slightly exothermic and releases some heat. Calculations of energy balances followed equations in table 3. From the energy balance, the energy conversion efficiency of CH_4 to H_2 was calculated dividing the energy value of the produced H_2 by the energy value of the consumed CH_4.

Table 3. Equations for energy balances of SMR and WGS processes.

SMR reaction	**WGS reaction**
$CH_4 + H_2O + \text{heat} \rightarrow CO + 3H_2$	$CO + H_2O \rightarrow CO_2 + H_2 + \text{waste heat}$
$E_{CH_4} = x_{CH_4} \cdot LHV_{CH_4}$	$E_{CO} = x_{CO} \cdot LHV_{CO}$
$E_{CO} = x_{CO} \cdot LHV_{CO}$	$E_{H_2} = x_{H_2} \cdot LHV_{H_2}$
$E_{3H_2} = x_{3H_2} \cdot LHV_{H_2}$	$E_{\text{waste heat}} = E_{CO} - E_{H_2}$
$E_{heat} = (E_{CO} \cdot E_{3H_2}) - E_{CH_4}$	

4.2. Inventory and impact assessment

The life cycle of each H_2 colour was divided into fuelling and driving a fuel cell truck, H_2 production processes, production of feedstock and transportations of LNG and CO_2. Calculations were based on GHG emission data for each process. Detailed emission data and sources for each process are included in appendix I.

4.2.1. Fuelling and driving a FCEV

To calculate the AGTP, yearly GHG emissions were calculated for the different H_2 colours. First, the amount of H_2 (x_{H2}) required to cover the daily demand of fuel to replace diesel in heavy truck transportation in Sweden was calculated using equation 4. The fraction of diesel in the heavy truck transport was 92% (n_{diesel}) (Trafikverket 2020a), and the fuel consumption (fc) was calculated from 8 kg H_2/100 km, which was an assumption based on FCH JU & Berger (2017) and Fuel Cells Works (2019). The distance (d) was 4 176 057 770 km/ year and represented the annual distance driven by heavy trucks in Sweden (Trafikanalys 2020a).

$$x_{H2} = (n_{diesel} \cdot fc \cdot d)/365 \quad [\text{kg } CO_2/\text{day}] \qquad (4)$$

4.2.2. Production process inventory calculations

Grey H_2

The daily amount of CH_4 (x_{CH_4}) required to produce H_2 was calculated using equation 5. The input x_{H2} was used from equation 4. The energy conversion efficiency was 78% (n_{SMR}) and the higher heating values were HHV_{H2} = 141.9 MJ/kg and HHV_{CH4} = 55.5 MJ/kg (Nikolaidis & Poullikkas 2017).

$$x_{CH_4} = \frac{x_{H2} \cdot HHV_{H2}}{n_{SMR} \cdot HHV_{CH4}} \quad \text{[kg CH}_4\text{/day]} \tag{5}$$

In equation 6, the amount of natural gas required for the SMR process (x_{LNG}) was calculated. The fraction of CH_4 in Norwegian LNG was 92% (n_{LNG}) (Kuczyński et al. 2020).

$$x_{LNG} = \frac{x_{CH4}}{n_{LNG}} \quad \text{[kg LNG/day]} \tag{6}$$

The CO_2 emissions from the SMR process (x_{CO_2}) was calculated using equation 7, multiplying x_{CH_4} with the combustion relation of CO_2 and CH_4, which was calculated by dividing the molecular mass of CO_2 (m_{CO_2}) with the molecular mass of CH_4 (m_{CH_4}).

$$x_{CO_2} = x_{CH_4} \cdot \frac{m_{CO_2}}{m_{CH_4}} \quad \text{[kg CO}_2\text{/day]} \tag{7}$$

Total CO_2 emissions ($x_{CO_2\,Grey}$) were calculated using equation 8, adding x_{CO_2} to the emissions from electricity consumption, which was calculated by multiplying the electricity consumption ($E_{el\,SMR}$) with the emission factor of the Nordic residual mix ($f_{residual}$). The electricity consumption was multiplied with the daily amount of H_2 (x_{H2}).

$$x_{CO_2\,Grey} = x_{CO_2} + x_{H2} \cdot E_{el\,SMR} \cdot f_{residual} \quad \text{[kg CO}_2\text{/day]} \tag{8}$$

Blue H_2

Calculations for blue H_2 followed the grey H_2 calculations but included a CCS unit. The captured CO_2 (x_{CCS}) was calculated using equation 9, assuming CO_2 capture from the pre-combustion stream containing 60% of the total CO_2 emissions ($n_{pre-comb}$), with 90% capture efficiency (n_{CCS}). The variable $x_{CO_2}$was calculated using equation 7.

$$x_{CCS} = n_{CCS} \cdot x_{CO_2} \cdot n_{pre-comb} \quad \text{[kg CO}_2\text{/day]} \tag{9}$$

Total GHG emissions for blue H_2 were calculated using equation 10, subtracting the captured CO_2 (x_{CCS}) and adding the emissions from heat ($x_{CO_2\,heat_{CCS}}$) and electricity ($x_{CO_2\,el_{CCS}}$) consumption of the CCS unit. The electricity consumption was 0.196 kWh/kg CO_2 and the thermal energy required was 0.083 kWh/kg H_2 (IEAGHG 2010).

$$x_{CO_2\,Blue} = \left(x_{CO_2\,Grey} - x_{CCS}\right) + x_{CO_2\,el_{SMR}} + x_{CO_2\,el_{CCS}} + x_{CO_2\,heat_{CCS}} \quad \text{[kg CO}_2\text{/day]} \tag{10}$$

Beige- and orange H_2

Calculations for beige and orange H_2 followed the grey and blue H_2 calculations but changing the natural gas feedstock to biomethane. The CH_4 composition of biomethane was 97% (n_{bioC}) (Uppsala Vatten 2018) and $x_{CH_4}$was calculated using equation 5. The required amount of biomethane (x_{bioC}) was calculated using equation 11.

$$x_{bioC} = \frac{x_{CH_4}}{n_{bioCH4}} \quad \text{[kg bioCH}_4\text{/day]} \tag{11}$$

Total GHG emissions for beige H_2 were the same as for grey H_2, calculated using equation 8, and emissions from orange H_2 were the same as for blue H_2, calculated using equation 10. However, the CO_2 emissions of beige and orange H_2 were considered biogenic, and the CO_2 uptake was accounted for in the biomethane production calculations.

The total share of available beige and orange H_2 (y) was calculated using equation 12. The yearly production of biogas in Sweden was divided by the yearly amount of biogas required to produce H_2 to cover the entire share of diesel in the heavy truck transportation. The annual production volume of biogas was 2044 GWh (V), with 47% produced from co-digestion plants (n_{codig}) and 35% from wastewater treatment plants (n_{WWT}) (Klackenberg 2020).

$$y = \frac{V \cdot (n_{codig} + n_{WWT})}{HHV_{CH_4} \cdot 10^{-6} \cdot 365 \cdot x_{bioCH_4}} \cdot 100 \quad [\%] \tag{12}$$

Green H_2

Green H_2 has no other GHG emissions than from the electricity production, which was calculated by multiplying the electricity consumption of 54.18 kWh/kg H_2 (E_{el}) (Valente et al. 2020), with the emission factor of wind power which was 15 g CO_2-eq/kWh (f_{wind}) (Gode et al. 2011). For electricity production, CH_4 and N_2O emissions were neglected, and the total CO_2 emissions were calculated using equation 13.

$$x_{CO_2Green} = f_{wind} \cdot E_{el} \cdot x_{H_2} \quad \text{[kg CO}_2\text{/day]} \tag{13}$$

The energy conversion efficiency (η_{green}) was calculated using equation 14, with HHV_{H_2}= 39.4 kWh/kg H_2 (Engineering ToolBox 2003).

$$\eta_{green} = \frac{HHV_{H_2}}{E_{el}} \cdot 100 \quad [\%] \tag{14}$$

4.2.3. Production of feedstock

Natural gas

The GHG emissions from the natural gas production were based on already existing well-to-tank (WTT) data from an LCA study of Norwegian LNG. The study was performed by Thinkstep (2017), on behalf of the Natural & Biogas Vehicle Association in Europe. The study covers the LNG supply to Central Europe, with Norway as main producer. Data for production, processing and liquefaction were taken from Thinkstep (2017), and calculations for LNG distribution were performed according to the methodology presented in section *4.2.4. Transportation of LNG and CO$_2$.* The GHG emissions from production, processing and liquefaction covered 77% (n_{WTT}) of the total WTT emissions with the emission factors of x_{CO_2}=10.90 g CO$_2$-eq/MJ$_{LHV}$, x_{CH_4}=2.30 g CO$_2$-eq/MJ$_{LHV}$ and x_{N_2O}=0,19 g CO$_2$-eq/MJ$_{LHV}$ (Thinkstep 2017). The heating value of natural gas was LHV_{NG}=46.5 MJ/kg (Antonini et al. 2020). Calculations for each gas were performed using equation 15.

$$x_{GHG} = x_{(CO_2,CH_4,N_2O)} \cdot LHV_{NG} \cdot n_{WTT} \quad \text{[g CO}_2\text{-eq/kg LNG]} \qquad (15)$$

Daily GHG emissions for the WTT process of LNG was calculated by multiplying the emission factors of each gas with the daily amount of LNG used to produce H$_2$ (x_{LNG}), calculated according to equation 6.

Biomethane

The GHG emissions from biomethane production, including upgrading, were based on an existing LCA study of Florio et. al (2019) and verified with data from Zahng et. al (2020) and Holmgren et. al (2015). The volume of biogas (V_{bioCH}) used to produce the required amount of biomethane for beige and orange H$_2$ was calculated using equation 16, where x_{bioCH_4} was calculated using equation 11. The lower heating value used was LHV_{bioCH4}=45.4 MJ/kg (Antonini et al. 2020) and the energy content was E_{bioCH4}=9.67 kWh/m^3 bioCH$_4$ (Svenskt gastekniskt center 2012). The conversion factor from kWh to MJ is 3.6.

$$V_{bioC} \quad = \frac{x_{bioCH_4}}{(E_{bioC} \quad \cdot 3.6/LHV_{bioC} \quad)} \quad \text{[m}^3\text{ bioCH}_4\text{/day]} \qquad (16)$$

The WTT emissions from biomethane production and upgrading was 0.58 kg/m^3 biogas (x_{CO_2WTT}) and the biomethane production rate was 0.62 m^3 bioCH4/m^3 biogas (η_{bioCH4}) (Florio et al. 2019). Further, the CO$_2$ emissions from biomethane ($x_{CO_2biomethane}$) were considered biogenic, which was counted for by including negative emissions when bound into the biomass. The negative biomass CO$_2$ emissions ($x_{biomass}$) were calculated using equation 17, with V_{bioCH4} calculated from equation 16 and $x_{CO_2}$from equation 7.

$$x_{biomass} = -1 \cdot (V_{bio} \quad \cdot x_{CO_2WTT}/\eta_{bioCH} \ + x_{CO_2}) \quad [\text{kg CO}_2/\text{day}] \qquad (17)$$

The total CO_2 emissions ($x_{CO_2biomethan}$) for biogas production and upgrading was calculated according to equation 18, with an electricity consumption of 0.33 kWh/m^3 biogas (E_{biogas}).

$$x_{CO_2biomethane} = (x_{CO2\,WTT}/\eta_{bioCH} \ ) \cdot V_{bioCH4} + x_{biomass} + (E_{biogas}/\eta_{bioCH4}) \cdot V_{bioCH4} \cdot f_{residual} \quad [\text{kg CO}_2/\text{day}] \qquad (18)$$

The CH_4 emissions were dependent on the leakage rate from production and upgrading of biogas, and was calculated based on an assumed leakage rate of 1.4% (l_{CH4}) (Holmgren et al. 2015) and a CH_4 content (n_{CH4}) of 97% in biomethane (Uppsala Vatten 2018). Total CH_4 emissions ($x_{CH_4biomethan}$) were calculated using equation 19, with x_{bioCH_4} calculated using equation 11.

$$x_{CH_4biomethan} \ = n_{CH4} \cdot l_{CH4} \cdot \mathrm{x}_{\mathrm{bioCH}_4} \quad [\text{kg CH}_4/\text{day}] \qquad (19)$$

The N_2O emissions from biogas production and upgrading were not included, based on recommendations in Florio et al. (2019) and Ardolino et al. (2020).

4.2.4. Transportation of LNG and CO_2

Transportation of LNG

The number of ships (N_{ships}) required to transport the daily amount of LNG that was needed for H_2 production, was calculated using equation 20. The daily LNG supply (x_{LNG}) was calculated using equation 6, and the ship size was assumed to be 7500 tonne/ship (x_{ship}), based on data from Gode et al. (2011).

$$N_{ships} = \frac{x_{LNG}}{x_{ship}} \quad [\text{no. ships/day}] \qquad (20)$$

The fuel consumption (*fc*) was 0.21 MJ/tonne-km (Gode et al. 2011). The distance (d) from Risavika to Nynäshamn on a roundtrip journey was 2626 km (Sea-distances 2021). The emission factors from production, distribution and usage of bunker oil were: $x_{CO \ \ bunker\ oil} = 85.7$ g CO_2/ MJ fuel, $x_{CH4\,bunker\ oil} = 0.0074$ g CH_4/ MJ fuel and $x_{N2O\ bunker\ oil} = 0.0038$ g CH_4/ MJ fuel (Gode et al. 2011). The total GHG emissions for LNG shipping were calculated from equation 21, for CO_2, CH_4 and N_2O respectively.

$$x_{GHG\,ship} = x_{ship} \cdot fc \cdot d \cdot x_{GHG\,bunkeroil} \ \cdot N_{ships} \quad [\text{kg CO}_2\text{,CH}_4\text{,N}_2\text{O/day}] \qquad (21)$$

For truck transport from Nynäshamn to Uppsala, the number of trucks (N_{trucks}) required to transport the daily amount of LNG (l_{CH}) was calculated using equation

22, with a truck size assumed to be 60 tonnes/truck (x_{truck}), based on heavy trucks (Transportstyrelsen 2020).

$$N_{trucks} = \frac{x_{LNG}}{x_{truck}} \quad \text{[no. trucks/day]} \qquad (22)$$

The fuel consumption for a diesel truck was 33.2 l/100 km (fc_{diesel}) (Trafikverket 2020a) and the density of diesel was 0.8 kg/l (ρ_{diesel}) (Neste Corporation 2020). The emission factors from production, distribution and usage of diesel with 5% RME were $x_{CO2\ diesel}$= 75.92 g CO_2/MJ fuel, $x_{CH4\ diesel}$= 0.030 g CH_4/MJ fuel and $x_{N2O\ diesel}$= 0.0022 g CH_4/MJ fuel. The heating value was LHV_{diesel} = 43.1 MJ/ kg fuel (Gode et al. 2011) and d = 260 km was the road distance of a roundtrip journey from Nynäshamn to Uppsala. The total GHG emissions for LNG truck transport ($x_{GHG\ truck}$) were calculated from equation 23, for CO_2, CH_4 and N_2O respectively.

$$x_{GHG\ truck} = fc_{diesel} \cdot \rho_{diesel} \cdot LHV_{diesel} \cdot d \cdot x_{diesel} \cdot N_{trucks}$$
$$\text{[kg } CO_2, CH_4, N_2O\text{/day]} \qquad (23)$$

Transportation of CO_2

The number of trucks required to transport the daily captured CO_2 (x_{CCS}) was calculated using equation 22, but with x_{CCS} (equation 9) instead of x_{LNG}. Further, the GHG emissions of truck transport of CO_2 were calculated using equation 23, with $d = 912\ km$.

The number of ships required to transport the CO_2 captured each day (x_{CCS}) was calculated from equation 20, but with x_{CCS} (equation 9) replacing x_{LNG}. Moreover, the GHG emissions from shipping the captured CO_2 were calculated from equation 21, with $d = 1296\ km$.

4.2.5. Emission summary

When the daily GHG emissions were calculated for each colour, it was divided by the yearly road performance of heavy trucks in Sweden in 2019, which was 410 180 000 000 tonne-km/year (Trafikanalys 2020a).

Additionally, diesel was used as a reference fuel for a heavy truck and was calculated using equation 24, with d = 4 176 057 550 km, representing the yearly distance driven by heavy trucks in Sweden.

$$x_{GHG\ truck} = fc_{diesel} \cdot \rho_{diesel} \cdot LHV_{diesel} \cdot d \cdot x_{diesel} \quad \text{[kg } CO_2, CH_4, N_2O\text{/day]} \qquad (24)$$

4.3. Time-dependent calculations

Future scenarios were created for different H_2 production deployments over 30 years. The scenarios were based on a literature review of the transportation sector and a market analysis of H_2 deployment, which is included in *3.2. Hydrogen in future heavy truck transportation.* The daily GHG emissions calculated in *4.2.5. Emission summary,* were multiplied with 365 to get annual emissions for CO_2, CH_4 and N_2O. The annual GHG emissions of each colour were used to form the future scenarios, with different deployment rates of the H_2 colours.

The future scenarios were illustrating the diesel displacement with H_2 for heavy trucks. The deployment rate of H_2 was based on a market analysis with assumptions based on FCH JU (2019), IRENA (2020) and Navas-Anguita et al. (2020). When the future scenarios were formed, the impact on the global mean surface temperature change from the emissions were calculated and evaluated over a period of 100 years. The theory behind time-dependent calculations is included in appendix II, and future emission scenario vectors are included in appendix III.

4.4. Sensitivity analysis

A sensitivity analysis was performed to test the impact of different assumptions made in the thesis by changing one parameter at a time. The sensitivity parameters were chosen based on the results in table 4. First, the electricity source for H_2 production was changed, from the Nordic residual mix to hydro and wind power. Second, the CH_4 leakage rate was changed to half, double, and four times the leakage rate. Third, the CO_2 capture rate was changed from pre-combustion capture to post-combustion capture, and for both pre- and post-combustion capture.

5. Results and analysis

In this section, the mass and energy balances are presented, followed by the climate impact of different H_2 production processes. Further, the time-dependent results of implementing H_2 in the transportation sector are shown, and finally, the results of the sensitivity analysis are illustrated and explained.

5.1. Mass- and energy balances

The mass balances for the SMR and WGS processes are shown in figure 9, assuming 1 kg of CH_4 entering the reformer. The SMR process requires similar amounts of CH_4 and H_2O. However, the mass conversion of H_2 is only 19% whereas 81% is converted to CO. For the WGS process, H_2O is needed again to convert CO into H_2. For this process, only 4% becomes H_2 while 96% is converted into CO_2. If considering the total SMR and WGS process, H_2 only represents 16% of the total mass output from the system. The remaining output is composed of 84% CO_2, which illustrates the carbon intensity of the process.

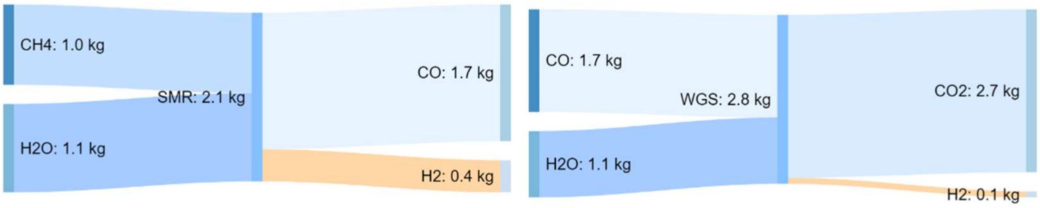

Figure 9. Theoretical mass balance of the SMR-WGS process

The theoretical energy balances for the SMR and WGS processes are illustrated in figure 10. The SMR process is an endothermic reaction and requires a relatively high amount of external heat. The WGS process is slightly exothermic with some waste heat as by-product from the reaction. The energy content of H_2 in the SMR process is 72% of the energy input, and 28% is found in the CO. For the WGS process, 86% is converted into H_2 while 14% becomes waste heat. Considering the total SMR and WGS system, H_2 represents 96% of the total energy input, and only 4% becomes waste heat. Such characteristics illustrate the energy efficiency of the SMR-WGS process.

Figure 10. Theoretical energy balance of the SMR-WGS process

For AEL water-electrolysis, the theoretical mass balance is shown in figure 11, assuming 1 kg of H_2O as input. Only 10% of the mass input becomes H_2 while 90% becomes O_2. However, the theoretical electricity conversion efficiency is shown in the energy balance (figure 12) in which H_2 has an energy conversion efficiency of 72% while 28% becomes heat. Here, the high energy content of H_2 is illustrated.

Figure 11. Mass balance for green H_2.

Figure 12. Energy balance for green H_2.

5.2. Climate impact of H_2

Here, the climate impact of the H_2 colours and future scenarios are presented. The different fuels are compared to a diesel reference, based on their GWP_{100}. Further, the climate impact due to AGTP for different H_2 colours and the future scenarios are presented.

5.2.1. Comparison of H_2 colours

The carbon footprint of the different H_2 colours are presented in table 4. The values represent WTT emissions per produced kg H_2 before it has been used as fuel for the heavy truck transport. Grey H_2 contributes with most emissions due to using natural gas as feedstock. The sub processes show that the SMR process contributes with 84% to total emissions. The feedstock production of natural gas consists of 14% and transportation of LNG between Norway and Sweden only consists of 2% of the total CO_2-equivalents for grey H_2. Blue H_2 contributes with lower emissions than grey H_2 due to CCS implementation. For blue H_2, the SMR process contributes with 72% to total emissions, which is a result of the captured CO_2. For beige and orange

H_2, the GHG emissions are biogenic which is shown as negative emissions from the feedstock production and positive emissions from the SMR process. It is shown that both the biogas production and SMR process have large impacts on the total GWP for beige and orange H_2. For green H_2, the electricity source is shown to contribute with 100% of the impact. The impact that the different sub processes have on the total impact for each H_2 colour was used as a base to choose parameters for the sensitivity analysis.

Table 4. Carbon footprints in CO_2-equivalents from different H_2 colours. The total CO_2-equivalents are first presented, followed by the emissions from the different processes.

[g CO_2-eq/kg H_2]	**Grey H_2**	**Blue H_2**	**Beige H_2**	**Orange H_2**	**Green H_2**
Total emissions	11.77	7.65	2.96	-1.16	0.83
Feedstock production	1.70	1.70	-6.91	-6.91	0.83
Transportations	0.18	0.46	-	0.28	-
SMR/ electrolysis	9.87	5.48	9.87	5.48	-

The climate impact of the GHG emissions, using GWP_{100} to convert gases to CO_2-equivalents, is presented in figure 13. Data for WTW values and sources are included in appendix I. Heavy fuel cell (FC) trucks that are fuelled with grey H_2 have the highest GHG emissions of the assessed H_2 colours, with only 2% lower emissions than a conventional internal combustion (IC) diesel truck. Even though FCEVs result in large improvements for air quality due to their zero emissions characteristic in terms of climate impact, their benefits are marginal compared to IC diesel trucks. Larger improvements can be seen when adding CCS to the system. Heavy FC trucks fuelled with blue H_2 contributes with 36% lower emissions than a conventional diesel truck. If natural gas is replaced with biomethane, the emissions are reduced further, as beige H_2 emits approximately 75% less than a conventional diesel truck. Orange H_2 generates net-negative emissions and contributes to an emission reduction of approximately 110% compared to a diesel truck. This means that heavy FC trucks provide a service of removing CO_2 from the atmosphere while being on the road. Heavy FC trucks that are fuelled with green H_2 are close to being climate neutral with an emission reduction of approximately 95% compared to diesel trucks. However, this result is only valid for wind power as electric source in the green H_2 production. Even though heavy FC trucks have higher efficiencies than a conventional IC diesel truck, the production process of H_2 has a large influence on the overall climate impact.

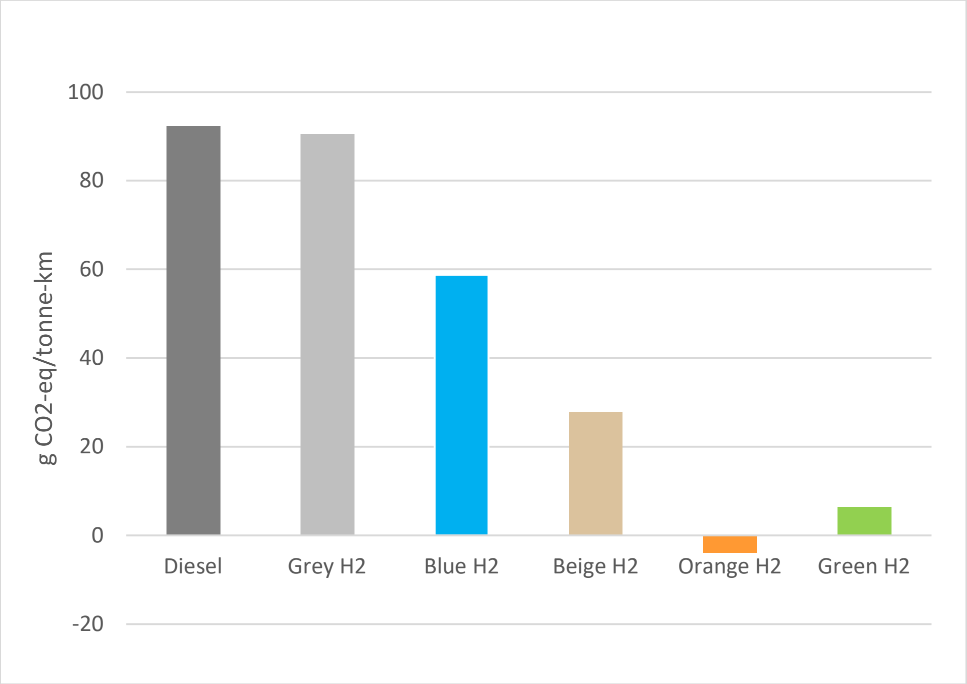

Figure 13. GWP_{100} values of diesel as reference fuel, compared to the different H_2 colours.

The temperature change for the assessed H_2 colours is illustrated in figure 14, for 30 years of H_2 production and evaluated over a 100 year time period. Both grey and blue H_2 contribute to a temperature increase that does not reach back to the initial temperature after 100 years. This is due to the additional carbon that grey and blue H_2 contribute with to the atmosphere. The temperature response from beige H_2 increases over the first 30 years and after that it decreases back to almost reach the initial temperature state. The temperature change from beige H_2 has a different behaviour than grey and blue H_2 which is a consequence of the high leakages of CH_4 from the biogas upgrading process. After 30 years, when the H_2 production process ends, the CH_4 emissions decompose relatively fast and do not affect the climate anymore. The temperature then begins to decrease back towards its initial temperature. Since orange H_2 is also affected by CH_4 leakages, the temperature response follows a similar pattern as for beige H_2. However, the temperature decreases below its initial state after 30 years, which is a result of removing CO_2 from the atmosphere. For green H_2, the temperature response is only slightly affected due to small emissions from wind power production. Again, this result of climate neutrality that green H_2 provides is only valid when wind power is used as the electricity source.

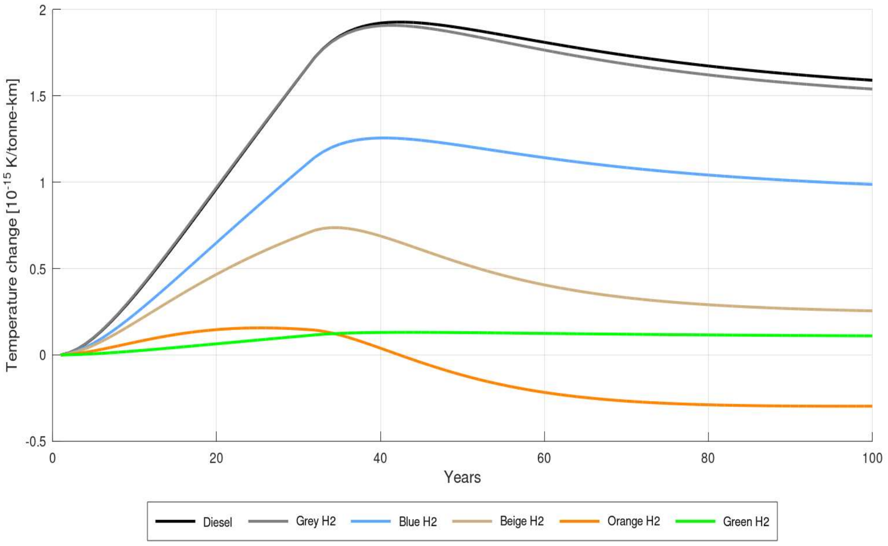

Figure 14. Temperature responses for grey, blue, beige, orange and green H_2.

5.2.2. Future scenarios

The temperature changes of the future scenarios with H_2 implementation in the heavy truck transport are illustrated in figure 15. The temperature changes are evaluated over a 100 year time horizon, which is the response to the GHG emissions from H_2 during a 30 years operation period.

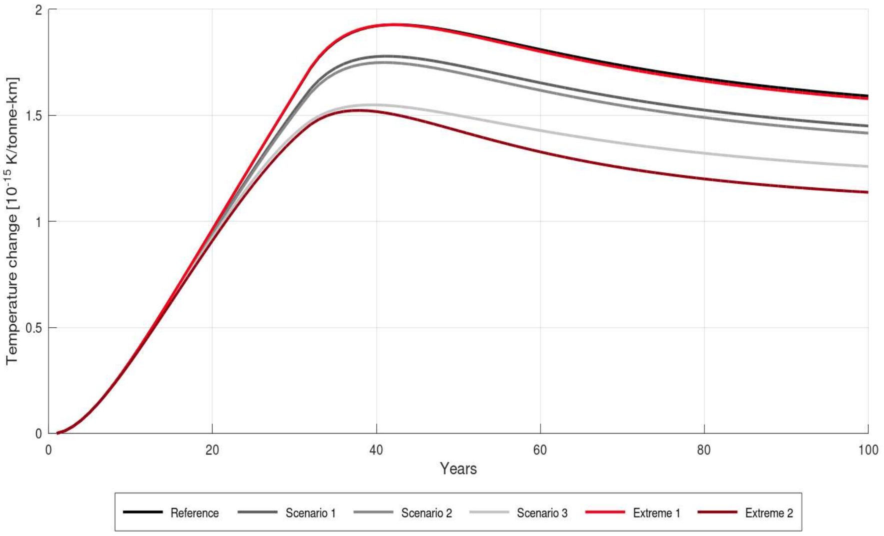

Figure 15. Temperature responses of the reference scenario and for five different future scenarios, including two extreme scenarios.

The reference scenario includes heavy conventional IC trucks fuelled with diesel only, while extreme scenario 1 shows grey H_2 implementation. The reference scenario and extreme scenario 1 show similar temperature responses throughout the 100 year period. It is not surprising that these two scenarios follow the same pattern as the carbon footprint of heavy IC diesel trucks and heavy FC trucks from grey H_2 are marginal, as seen in figure 13. From this result, extreme scenario 1 seems to be the worst-case scenario for H_2 implementation for heavy truck transportation.

Further, scenario 1 represents a natural gas dominant scenario, where diesel is displaced with grey and blue H_2. The temperature response is reduced with approximately 10% after 40 years and follows the same reduction throughout the 100 years period, compared to the reference scenario. The reduction is a consequence of the captured CO_2 that blue H_2 provides. The reduction in scenario 2 is larger compared to the reference scenario, which is due to beige and orange H_2 implementation. However, the highest share of beige and orange H_2 was calculated to cover only 10% of the total diesel share for heavy trucks in Sweden, which does not affect the temperature response significantly. After 40 years, the temperature increase starts to decline and after 100 years the temperature increase is approximately 12% lower than in the reference scenario. Scenario 3 represents a mix of all H_2 colours and could be the most likely case in Sweden. The share of green H_2 increases while blue H_2 decreases which results in a 21% temperature reduction compared to the reference scenario. The same pattern of temperature response follows throughout the 100 years period. When comparing scenario 2 and scenario 3 it is shown that a high share of green H_2 in combination with beige and orange H_2 contributes to lower climate impact than for H_2 production through SMR with natural gas.

Extreme scenario 2 represents diesel displacement with orange H_2 and the temperature response is seen to behave differently from the other scenarios. The first 30 years, the temperature increases rapidly and reaches a reduction of 22% compared to the reference scenario. However, after 38 years, the temperature begins to decline in a faster rate than the other scenarios and after 100 years it has reached a 30% reduction in temperature increase compared to the reference scenario. The behaviour of the temperature response for extreme scenario 2 is similar to orange H_2 in figure 14. The high CH_4 leakage that biogas production and upgrading emits decomposes relatively fast and does not impact on the climate anymore. That is when the temperature starts to decrease and move towards its initial temperature state. Extreme scenario 2 can be seen as the best-case scenario for H_2 implementation, due to the lowest AGTP. Although orange H_2 itself could contribute with negative temperature changes due to the bio-CCS technology, it does not reach negative emissions when it is implemented in combination with diesel. This result shows the importance of combining H_2 implementation with other renewable fuels to phase out fossil diesel in a faster rate.

5.3. Sensitivity analysis

The results in table 4 show that feedstock production, including biomethane, natural gas and electricity, combined with the SMR process have large impacts on total emissions. The sensitivity of the system was calculated and represented in figure 16, 17 and 18, by changing electricity source, methane leakage for natural gas and biomethane production as well as CO_2 capture rate for the SMR process with CCS.

The thesis assumption of the electricity source represents the Nordic residual mix in the SMR process for grey, blue, beige and orange H_2 while the electrolytic process for green H_2 is produced from wind powered electricity. When changing the electricity source to the Nordic residual mix even for the electrolytic process, it shows to have an extremely high impact on green H_2. A heavy FC truck fuelled with green H_2 from the Nordic residual electricity mix reaches emissions that are 53% higher than what a conventional diesel truck would emit. This parameter shows that the system of green H_2 is highly sensitive to the electricity source. However, the choice of electricity source used in the SMR process of grey, blue, beige and orange H_2 has a smaller impact.

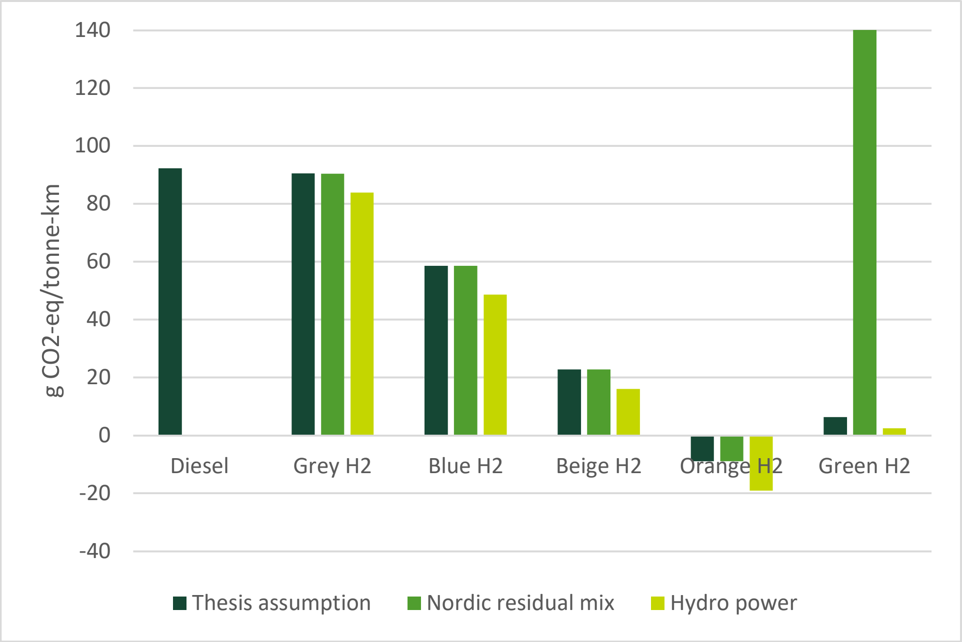

Figure 16. The system's sensitivity of the electricity source, due to changes between the thesis assumption, the Nordic residual mix, and hydro power. Diesel is used as a reference parameter when comparing the emission output of the H_2 colours.

The sensitivity of the system due to CH_4 leakages in feedstock production of natural gas and biomethane is presented in figure 17. The most sensitive systems are beige and orange H_2 due to biomethane production. The negative emissions of orange H_2 increases when reducing the CH_4 leakages to 0.7%. If the CH_4 leakage rate approaches 3%, orange H_2 does no longer generate negative emissions. This consideration is important when promoting orange H_2 as a fuel that provides a service of negative emissions.

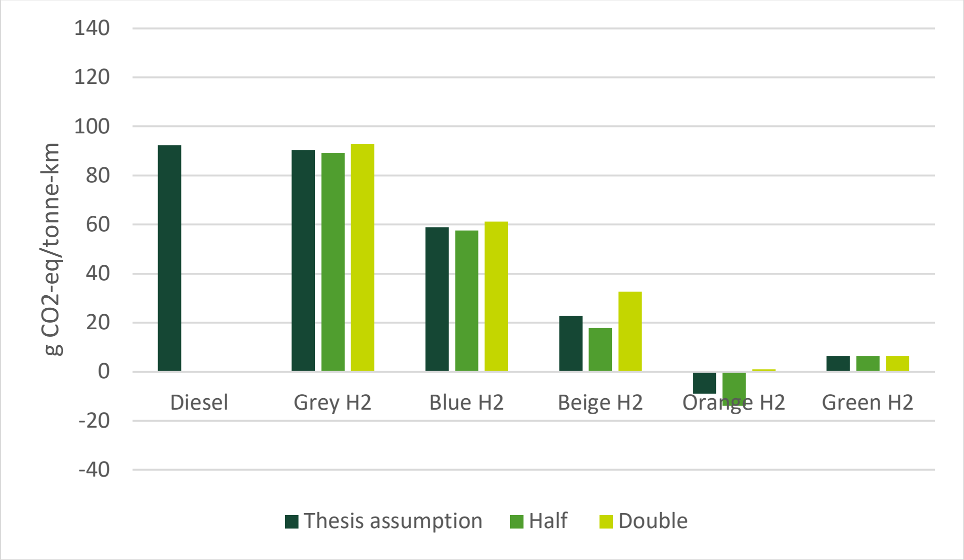

Figure 17. The system's sensitivity of CH_4 leakages in natural gas and biomethane production, due to changes between the thesis assumption of 1.4% leakage to 0.70% and 2.8%. Diesel is used as a reference when comparing the emission output of the H_2 colours.

The sensitivity of the system due to the performance of the CCS unit in connection to the SMR plant is shown in figure 18, where blue and orange H_2 are the only colours that are affected by this parameter. The thesis assumption represents CO_2 capture at the pre-combustion stream which covers 54% of the entire CO_2 emissions. However, if the CO_2 capture site is located at the post-combustion stream, the capture rate covers 36% of the total CO_2 emissions and orange H_2 does no longer generate negative emissions. If the CCS unit instead would cover CO_2 capture from both the pre- and post-combustion streams, 90% of the total CO_2 could be captured and the net-negative emissions will drop three times lower than for only pre-combustion capture. Even though blue and orange H_2 improve their climate impact when expanding the CO_2 capture rate, the economic costs increase with a more diluted CO_2 stream as well as with multiple CO_2 capture sites.

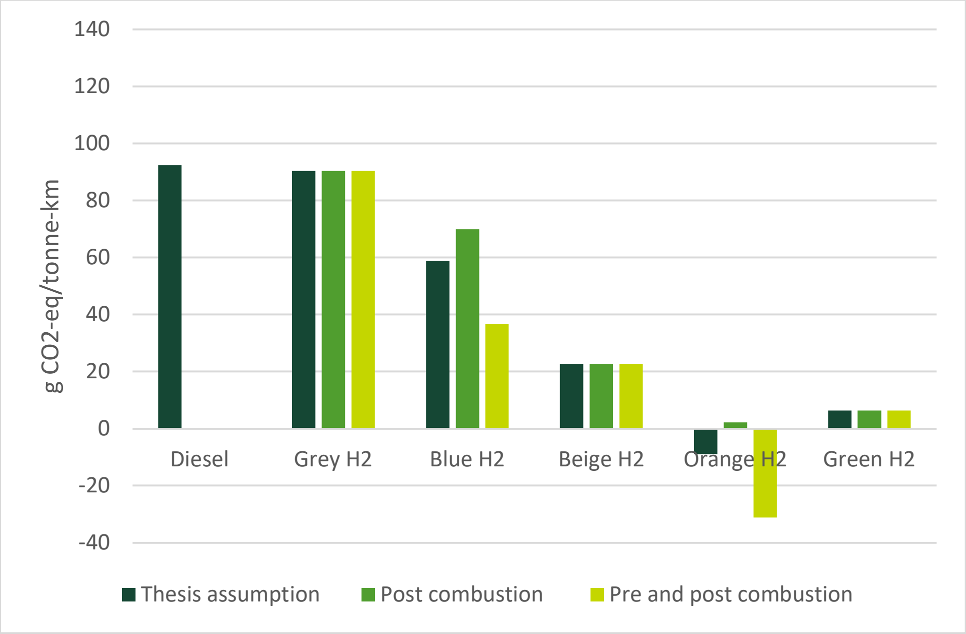

Figure 18. The system's sensitivity of CO_2 capture rate in the CCS process, due to changes between the thesis assumption to post-combustion capture and to pre- and post-combustion capture. Diesel is used as a reference when comparing the emission output of the H_2 colours.

6. Discussion

As a new energy market is about to develop due to H_2 implementation, the supply and demand must go hand in hand. The transportation sector faces challenges reducing its climate impact. Hydrogen as a fuel in FCEVs could potentially displace fossil fuels, with water as the only direct emission. However, there are only a few FCEVs on the market today, and the demand remains low. The low demand could be a result of low supply combined with poor infrastructure for fuel stations, which could contribute to an increased demand for BEVs instead. However, if the demand for FCEVs remains low, the supply will most likely remain low as well, which makes it challenging for H_2 to be implemented on the market.

The technology of producing H_2 is already developed, and as seen in this study, the climate impact varies a lot depending on production technology. However, the technology costs increase as the climate impact decreases, which is another challenge of implementing H_2 on the market. Grey H_2 is already at the state of commercialization and is the cheapest H_2 on the market, although it contributes with the highest emissions. If adding CCS to the H_2 production process, emissions decrease while prices increase. However, both grey and blue H_2 could work as bridge solutions to implement H_2 on the market. When the demand increases, the technology and investment prices will likely fall which could give space to more sustainable technologies such as beige, orange and green H_2.

The most climate beneficial H_2 colours are orange and green H_2. Orange H_2 that are produced from biomethane meets limitations due to the biogas production. Also, biogas vehicles are already in commercial use, commonly as trucks or city buses, which makes biomethane based H_2 competitive with other biogas vehicles. However, the European commission has proposed a requirement of zero-emissions from the exhaust pipe of all cars by 2026 (Avfall Sverige 2021), which would threaten the development of biogas vehicles. If this proposal would go through, FCEVs fuelled with beige and orange H_2 could be a solution to continue the usage of the biogas that is available in Sweden. Another motivation for orange H_2 implementation could be if aid schemes for bio-CCS would be regulated. The Swedish Energy Agency (sv. Energimyndigheten) has proposed a framework of a reversed auction aid for bio-CCS. In the proposal, the reversed auction is planned to be implemented in 2022 and would work as an economic support for investments and operations of bio-CCS (Energimyndigheten 2021). If orange H_2 could expect to receive payments for its service of generating negative emissions, implementations could be motivated.

Green H_2 from renewable electricity was shown to be a climate neutral alternative as a fuel for the transportation sector. Although it is highly sensitive to the electricity source that is used, green H_2 can have further advantages of being connected to an intermittent power production plant. If green H_2 is connected to wind or solar power plants, it could produce H_2 from excess electricity and work as an energy storage to balance the electric grid. However, the expensive investment and operational costs of green H_2 challenge its implementation and support schemes are crucial for green H_2 development as well.

6.1. Sources of uncertainty

Several assumptions were made in this study which can cause uncertainties in the results. In the future scenarios, the total amount of H_2 was assumed to be produced in Uppsala, due to the transportation distances. Also, the truck transportation of LNG and captured CO_2 was calculated to be between 50-70 trucks per day. This result is not realistic and if multiple production sites as well as buffer storages would have been considered, the result would probably be more realistic. Another reason for the high number of daily trucks is because they were calculated to cover 100% of the diesel displacement in this study. Diesel displacement reaches 82% as the highest H_2 implementation rate. However, according to table 4, transportations do not have a large effect on the result which shows that this parameter does not have a major impact on uncertainty. Another source of uncertainty could come from the future scenarios, where no renewable diesel is considered. If fossil diesel would be mixed with other renewable fuels, the AGTP of the heavy truck transport from the different future scenarios would likely decrease.

6.2. Sustainability aspects

Biogas is considered a renewable energy source, and the CO_2 emissions are biogenic, being part of the fast carbon cycle. In this study, biogenic CO_2 emissions are calculated with GWP_{100} as zero. However, aspects such as growth time of a forest and the nutrition in the soil are affected by biogas production. Also, the CH_4 leakage from the biogas upgrading unit has been shown to have major impacts on the climate. The environmental sustainability of biogas production can vary a lot depending on the control of the CH_4 leakage that the biogas plants have.

Another sustainability consideration is the production capacity of the feedstock. The lowest climate impacts were seen from H_2 with biomethane as feedstock and wind powered electricity as energy source. Currently, the biogas production is limited by the organic waste which means that if all upgraded biogas is used for H_2

production, other processes that are fuelled with biogas would have to use other fuels. The sustainability aspect of beige and orange H_2 is therefore dependent on how other processes in the energy system will be affected by using biomethane as feedstock. Additionally, when displacing heavy diesel trucks in Sweden with a high share of green H_2, the demand of renewable electricity increases. The increasing demand of electricity will require extensions of the current power grid and perhaps also new constructions of wind power, which can affect the sustainability of green H_2.

The sustainability of CCS implementation is debated. While IEA (2021) expresses CCS as an important technology to reduce emissions and meet the global climate targets, Greenpeace claims that CCS cannot save the climate (Ash et al. 2015). Even though the debate is ongoing however CCS is seen as a sustainable solution or not, the technology can remove CO_2 from the atmosphere, which is crucial to reach the climate goals. On the other hand, CCS does not solve the problem itself, but only the consequences of it. However, we are currently at a point where urgent solutions must develop to counteract the climate changes and reach the climate goals, where CCS can be a key solution.

6.3. Future studies

This study provides a picture of how H_2 could contribute to a low-carbon transportation sector for heavy trucks. A suggestion for further investigations is to develop the future scenarios and include other renewable fuels such as FAME and HVO, and further assess the feasibility of electric roads for heavy trucks. If the diesel would be replaced with renewable fuels more rapidly, the emission profiles in the future scenarios could approach the net-zero target faster. Furthermore, it would be interesting to expand the scope and cover a larger part of the transportation sector, such as aviation and maritime transport.

Another suggestion of continuous studies is to assess the integration of CCS from the biogas upgrading unit, in combination with CO_2 capture from the SMR process. If CO_2 could be captured from both the biogas upgrading process and the H_2 production process, it could possibly result in a larger reduction of CO_2 from the atmosphere while net-negative emissions increase.

7. Conclusion

Hydrogen is a promising fuel for a future decarbonized transportation sector. Due to the high energy density of H_2, FCEVs do not require a heavy battery as for BEV, which makes H_2 a beneficial fuel for heavy truck transport. However, the production process can have a major impact on the environmental footprint of H_2. The CO_2-equivalent footprints due to the GWP_{100} for grey H_2 is only 2% lower than for a conventional diesel truck. If CCS is implemented to the SMR unit, as for blue H_2, the GWP_{100} is reduced by 36% compared to a diesel truck. When replacing natural gas with biomethane as feedstock, the emissions are reduced by 75%, as for beige H_2. If implementing CCS to the SMR process with biomethane as feedstock it becomes orange H_2 which results in net-negative emissions with a reduction of approximately 110% compared to a conventional diesel truck.

Grey and blue H_2, which are fossil based, can be used in regions with low natural gas prices, or act as a bridge solution to implement H_2 on the market. Beige and orange H_2 are good alternatives in regions with high biogas production and high political acceptance of CCS. In Sweden, beige and orange H_2 can cover a maximum share of 10% within heavy truck transport, due to the limited biogas production. In regions with low electricity costs and high availability of wind or solar power, green H_2 is a good alternative. However, in a future energy system with H_2 implementation, it will most likely require a mix between SMR based and water-electrolysis production.

The temperature change on Earth can increase between $1.6 \cdot 10^{-15}$ to $1.8 \cdot 10^{-15}$ K/tonne-km depending on the mix of H_2 colours that are implemented in a future heavy truck sector. The future scenarios with H_2 implementation contribute to a reduction in the temperature increase between 9% to 21% depending on the mix of H_2 colours, compared to diesel trucks. The highest temperature increase comes from diesel displacement with grey and blue H_2 while the lowest temperature increase results from a mix between all H_2 colours, but with a high share of green H_2. Although H_2 implementation in the heavy truck transport can contribute to a reduced climate impact, it is necessary to combine H_2 with other renewable fuels, as the predicted H_2 capacity looks today. To reach the Swedish national target of net-zero emissions by 2045, a higher share of renewable fuels, together with H_2, is most likely necessary. Hydrogen will be a good alternative in combination with other renewable fuels.

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Appendix I: LCA calculations

The emission data and LCA calculations are presented in this section. Each process step in the hydrogen lifecycle is defined and GHG emissions are described.

Natural gas production

Properties

Value	Unit	Description	Source
46.5	MJ/kg	LHV natural gas (LNG)	Antonini 2020
28	CO_2-eq	GWP CH_4	IPCC 2013
265	CO_2-eq	GWP N_2O	IPCC 2013

Production data

Value	Unit	Description	Source
10.90	g CO_2-eq/MJ (LHV)	EU Central: CO_2 emissions	Thinkstep 2017
2.30	g CO_2-eq/MJ (LHV)	EU Central: CH_4 emissions	Thinkstep 2017
0.10	g CO_2-eq/MJ (LHV)	EU Central: N_2O emissions	Thinkstep 2017
77%	-	GHG results of production, processing and liquefaction	Thinkstep 2017

Emissions natural gas production

Value	Unit	Description	Source
0.39	kg CO_2-eq/kg	CO_2 emissions from production, processing and liquefaction	Calculation
0.082	kg CO_2-eq/kg	CH_4 emissions from production, processing and liquefaction	Calculation
0.0036	kg CO_2-eq/kg	N_2O emissions from production, processing and liquefaction	Calculation

Output natural gas

Value	Unit	Description	Source
3009059	kg NG/ d	Natural gas required for H2 production per day	Calculation[1]
1174359	kg CO_2/ d	CO_2 emissions per day	Calculation[2]
8550	kg CH_4/ d	CH_4 emissions per day	Calculation[3]
40.66	kg N_2O/ d	N_2O emissions per day	Calculation[4]

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[1] Calculation input for grey and blue H_2

[2] Calculated values are verified with Gode et al. (2011) and Barnett (2010)

[3] ibid

[4] ibid

Biogas production

Properites biogas

Value	Unit	Description	Source
45.4	MJ/kg	LHV biomethane	Antonini 2020
97%	-	Fraction of CH_4 in upgraded biogas	Uppsala Vatten 2018
1.4%	-	CH_4 leakage rate	Holmgren et al. 2015

Biogas production + upgrading

Value	Unit	Description	Source
0.33	kWh/m^3 biogas	Mean value electricity consumption (PSA)	Calculation[5]
0.00	kWh/m^3 biogas	Heat consumption (PSA)	ibid
1228653	m^3 biogas/d	Biogas needed to produce bioCH_4	Calculation
1981698	kWh/d	Electricity consumption per day	Calculation
0.62	kg bioCH_4/m^3 biogas	Biomethane produced	Florio et al. 2019
-11079873	kg CO_2/d	CO_2 binded in biomass	Calculation, OrangeH2

Well-to-tank emissions

Value	Unit	Description	Source
0.58	kg/m^3 biogas	CO_2 emissions PSA upgrading	Florio et al. 2019[6]
0.015	kg/m^3 biogas	CH_4 emissions PSA upgrading	ibid[7]
0.00	kg/m^3 biogas	N_2O emissions PSA upgrading	ibid[8]
38769	kg CH_4/d	CH_4 leakage	Calculation[9]

Output biomethane

Value	Unit	Description	Source
2854883	kg/d	Biomethane required for H_2 production	Calculation[10]
-6926044	kg CO_2/d	CO_2 emissions per day	Calculation[11]
38769	kg CH_4/d	CH_4 emissions per day	Calculation[12]
0.00	kg N_2O/d	N_2O emissions per day	Calculation[13]

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[5] Calculation verified with Zhang et al. (2020) and Florio et al. (2019)

[6] Data verified with Ecoinvent 3.7.1

[7] ibid

[8] Data verified with (Ardolino et al. 2020)

[9] Calculation verified with Florio et al. (2019)

[10] Calculation input for beige and orange H_2

[11] Calculation verified with Gode et al. (2011) and Ecoinvent 3.7.1 (2020)

[12] Calculation verified with Gode et al. (2011) and (Ardolino et al. 2020)

[13] ibid

Grey H_2

Properties

Value	Unit	Description	Source
16.043	u	Molecular mass CH_4	Periodic table
44.011	u	Molecular mass CO_2	Periodic table
55.50	MJ/kg	HHV CH_4	Nikolaidis & Poullikkas (2017)
141.90	MJ/kg	HHV H_2	Nikolaidis & Poullikkas (2017)
0.084	kg/m^3	Density H_2 at NTP	Pacific Northwest National Laboratory (n.d.)
1.84	kg/m^3	Density CO_2 at NTP	Engineering ToolBox (2003)

Inflow SMR

Value	Unit	Description	Source
78%	-	SMR conversion efficiency	Valente et al. (2020)
2769237	kg CH_4/ d	CH4 required for x kg H_2/d	Calculation
3.3	kg CH_4/ kg H_2	CH_4/ H_2 ratio	Calculation
40	%	Fraction of natural gas to fuel	IEA (2019), Nikoaldis (2017)
60	%	Fraction of natural gas to feedstock	IEA (2019), Nikoaldis (2017)
3009059	kg NG/ d	Total amount of natural gas	Calculation
1203624	kg NG/ d	Amount of natural gas used as fuel	Calculation
1805435	kg NG/ d	Amount of natural gas used as feedstock	Calculation
92%	-	Fraction of methane in Norwegian LNG	Kucynski (2020)
2.6	kWh/kg H_2	Electricity consumption	Valente (2020)

Outflow SMR

Value	Unit	Description	Source
844822.16	kg H_2/ d	H_2 production hypthetical plant	Assumption input (calculation)
60	%	Fraction of CO_2 by feedstock	Antonini (2020)
40	%	Fraction of CO_2 by fuel	Antonini (2020)
2.74	-	Combustion relation of CO_2 from CH_4	Calculation
7596888.66	kg CO_2/ d	Total CO_2 emissions from CH_4	Calculation
4558133.19	kg CO_2/ d	CO_2 emissions from feedstock	Calculation
3038755.46	kg CO_2/ d	CO_2 emissions from fuel	Calculation
0.41	m^3 CO_2/m^3 H_2	Total CO_2 emissions	Calculation
8.99	kg CO_2/ kg H_2	Total amount of CO_2 per kg H_2	Calculation
5.40	kg CO_2/ kg H_2	Post-combustion CO_2 emissions	Calculation
3.60	kg CO_2/ kg H_2	Pre-combustion CO_2 emissions	Calculation
0.34	kg CO_2-eq/ kWh	Emission factor residual mix 2019	Energimarknadsinspektionen (2020)

Total inflow

Value	Unit	Description	Source
3009059	kg NG/ d	Total amount of natural gas	Calculation
2196538	kWh/ d	Total electricity needed for SMR	Calculation

Total outflow

Value	Unit	Description	Source
844822	kg H_2/ d	Produced H_2	Calculation
8340461	kg CO_2/ d	CO_2 emissions	Calculation[14]
0.00	kg CH_4/ d	CH_4 emissions	Calculation
0.00	kg N_2O/d	N_2O emissions	Calculation

Blue H_2

Same values as for grey H_2 are used but additionally, blue H_2 includes CO_2 capture. Data and calculations are provided in this section.

CCS inflow

Value	Unit	Description	Source
90	%	Fraction of CO_2 captured by the plant	Skagestad et al. (2017)
0.083	kWh/kg CO_2	Thermal energy required	IEAGHG (2010)
0.196	kWh/kg CO_2	Electricity for CO_2 capture and compression	ibid
4558133	kg CO_2/d	CO_2 emissions from feedstock	Calculation

CCS outflow

Value	Unit	Description	Source
4102320	kg CO_2/ d	Amount of CO_2 captured per day	Calculation
4.86	kg CO_2/kg H_2	Amount of CO_2 captured per kg H_2	Calculation
54	%	Fraction of CO_2 captured related to total CO_2 production	Calculation[15]

Total inflow

Value	Unit	Description	Source
3009059	kg NG/ d	Total amount of natural gas	Calculation
3341085	kWh/ d	Total electricity needed for SMR + CCS	Calculation

Total outflow

Value	Unit	Description	Source
844822	kg H_2/ d	Produced H_2	Calculation
4625593	kg CO_2/ d	CO_2 emissions	Calculation
0.00	kg CH_4/ d	CH_4 emissions	Calculation
0.00	kg N_2O/d	N_2O emissions	Calculation

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[14] Calculation verified with Valente et al. (2020) and Nikolaidis & Poullikkas (2017)

[15] Calculation verified with Antonini et al. (2020)

Beige and orange H_2

This section provides data and calculations for beige and orange H_2, which follows the same calculations except that orange H_2 includes a CCS step.

Properties

Value	Unit	Description	Source
16.043	u	Molecular mass CH_4	Periodic table
44.011	u	Molecular mass CO_2	Periodic table
55.50	MJ/kg	HHV CH_4	Nikolaidis & Poullikkas (2017)
141.90	MJ/kg	HHV H_2	Nikolaidis & Poullikkas (2017)
0.084	kg/m^3	Density H_2 at NTP	Pacific Northwest National Laboratory (n.d.)
1.84	kg/m^3	Density CO_2 at NTP	Engineering ToolBox (2003)
0.657	kg/m^3	Density CH_4	Engineering ToolBox (2003)
0.2777777778	-	Conversion MJ -> kWh	

Share of beige/ orange H_2

Value	Unit	Description	Source
47%	-	Codigestion plants biogas Sweden	Klackenberg (2020)
35%	-	Wastewater treatment plants	ibid
2044	GWh	Produced biogas in Sweden per year	ibid
1676	GWh/year	Biogas available from codigestion + WWT	Calculation
108718703	kg/year	Available biogas per year	Calculation
297860	kg/d	Available biogas per day	Calculation
10	%	Share of beige/ orange H_2 to cover heavy trucks	Calculation
844822	kg H_2/d	Amount of H_2 required to cover diesel heavy trucks	Calculation

Inflow SMR

Value	Unit	Description	Source
78	%	SMR conversion efficiency	Valente et al. (2020)
2769237	kg CH_4/ d	CH_4 required for x kg H_2/d	Calculation
3.28	kg CH_4/ kg H_2	CH_4/ H_2 ratio	Calculation
40	%	Fraction of natural gas to fuel	IEA (2019), Nikoaldis (2017)
60	%	Fraction of natural gas to feedstock	IEA (2019), Nikoaldis (2017)
2854883	kg/ d	Total amount of biomethane	Calculation
1141953	kg/ d	Amount of biomethane used as fuel	Calculation
1712930	kg/ d	Amount of biomethane used as feedstock	Calculation
97	%	Fraction of methane in biomethane	Uppsala Vatten (2018)
2.6	kWh/kg H_2	Electricity consumption	Valente (2020)

Outflow SMR

Value	Unit	Description	Source
844822	kg H_2/ d	Hydrogen production hypthetical plant	Assumption input
60	%	Fraction of CO_2 by feedstock	Antonini (2020)
40	%	Fraction of CO_2 by fuel	Antonini (2020)
2.74	-	Combustion relation of CO_2 from CH_4	Calculation
7596888.66	kg CO_2/ d	Total CO_2 emissions from CH_4	Calculation
4558133.19	kg CO_2/ d	CO_2 emissions from feedstock	Calculation
3038755.46	kg CO_2/ d	CO_2 emissions from fuel	Calculation
0.41	m^3 CO_2/m^3 H_2	Total CO_2 emissions	Calculation
8.99	kg CO_2/ kg H_2	Total amount of CO_2 per kg H_2	Calculation
5.40	kg CO_2/ kg H_2	Post-combustion CO_2 emissions	Calculation
3.60	kg CO_2/ kg H_2	Pre-combustion CO_2 emissions	Calculation
0.34	kg CO_2-eq/ kWh	Emission factor residual mix 2019	Energimarknadsinspektionen (2020)

CCS inflow

Value	Unit	Description	Source
90	%	Fraction of CO_2 captured by the plant	Skagestad et al. (2017)
0.083	kWh/kg CO_2	Thermal energy required	IEAGHG (2010)
0.196	kWh/kg CO_2	Electricity for CO_2 capture and compression	ibid

CCS outflow

Value	Unit	Description	Source
4102320	kg CO_2/ d	Amount of CO_2 captured per day	Calculation
4.86	kg CO_2/kg H_2	Amountt of CO_2 captured per kg H_2	Calculation
54	%	Fraction of CO_2 captured related to total CO_2 production	Calculated[16]

Total inflow

Value	Unit	Description	Source
2854883	kg/ d	Total amount of biomethane	Calculation
3341085	kWh/ d	Total energy needed for SMR + CCS	Calculation

Total outflow

Value	Unit	Description	Source
844822	kg H_2/ d	Produced H_2	Calculation
4625593	kg CO_2/ d	CO_2 emissions	Calculation
0.00	kg CH_4/ d	CH_4 emissions	Calculation
0.00	kg N_2O/ d	N_2O emissions	Calculation

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[16] Calculation verified with Antonini et al. (2020)

Green H_2

Properties

Value	Unit	Description	Source
141.9	MJ/kg	HHV H_2	Nikolaidis & Poullikkas (2017)
39.4	kWh/kg H_2	HHV H_2	Engineering ToolBox (2003)
0.084	kg/m^3	Density H_2 at NTP	Pacific Northwest National Laboratory (n.d.)
15.0	g/kWh el	CO_2 emissions to air from wind power. WTT	Gode et al. (2011)
0.00340	g/kWh el	CH_4 emissions to air from wind power. WTT	ibid
0.000500	g/kWh el	N_2O emissions to air from wind power. WTT	ibid
5.70	g/kWh	CO_2 emissions to air from hydropower. WTT	ibid
0.00400	g/kWh	CH_4 emissions to air from hydropower. WTT	ibid
0.0000920	g/kWh	N_2O emissions to air from hydropower. WTT	ibid
338.52	g CO_2-eq/ kWh	Emission factor residual mix 2019	Energimarknadsinspektionen (2020)

Inflow electrolyser

Value	Unit	Description	Source
54.18	kWh/kg H_2	Electricity consumption	Valente et al. (2020)
45772465	kWh/d	Electricity required per day	Calculation
73	%	Electrolyser conversion efficiency	Calculation[17]

Outflow electrolyser

Value	Unit	Description	Source
844822	kg H_2/ d	Produced H_2	Calculation
686587	kg CO_2/ d	CO_2 emissions	Calculation
156	kg CH_4/ d	CH_4 emissions	Calculation
23	kg N_2O/d	N_2O emissions	Calculation

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[17] Calculation verified with Valente et al. (2020)

Transportation

This section provides data and calculations for LNG and CO_2 transport on a round-way journey.

LNG: Ship Risavika port – Nynäshamn port

Value	Unit	Description	Source
6.7	g/MJ fuel	Bunker oil: CO_2 emissions WWT	Gode et al. (2011)
0.073	g/MJ fuel	Bunker oil: CH_4 emissions WWT	ibid
0.00015	g/MJ fuel	Bunker oil: N_2O emissions WWT	ibid
79	g/MJ fuel	Bunker oil: CO_2 emissions. TTW	ibid
0.00046	g/MJ fuel	Bunker oil: CH_4 emissions. TTW	ibid
0.0036	g/MJ fuel	Bunker oil: N_2O emissions. TTW	ibid
40.4	MJ/kg	LHV bunker oil	ibid
0.657	kg/m^3	Density CH_4	Engineering ToolBox (2003)
7500	ton/ship	Size of ship	Gode et al. (2011)
0.205	MJ/ton-km	Fuel consumption	ibid
1418	nautical miles	Sea distance Risavika – Nynäshamn roundtrip	Sea-distances (2021)
19.5	knots	Average speed	Laugen (2013)
4037684	MJ fuel/ship	Fuel consumption	Calculation
3009059	kg LNG/d	LNG required for daily H_2 production	Natural gas calculations
0.40	ships/d	Share of ships filled with LNG per day	Calculation
138830	kg/d	CO_2 emissions per day (roundtrip)	Calculation
119	kg/d	CH_4 emissions per day (roundtrip)	Calculation
6.1	kg/d	N_2O emissions per day (roundtrip)	Calculation

LNG: Truck Risavika port – Nynäshamn port

Value	Unit	Description	Source
6.32	g/MJ fuel	Diesel (5% RME): CO_2 emissions WWT	Gode et al. (2011)
0.0328	g/MJ fuel	Diesel (5% RME): CH_4 emissions WWT	ibid
0.00104	g/MJ fuel	Diesel (5% RME): N_2O emissions WWT	ibid
69.6	g/MJ fuel	Diesel (5% RME): CO_2 emissions TTW	ibid
0.00050	g/MJ fuel	Diesel (5% RME): CH_4 emissions TTW	ibid
0.0012	g/MJ fuel	Diesel (5% RME): N_2O emissions TTW	ibid
33.2	l/100 km	Fuel consumption diesel heavy truck	Trafikverket (2019)
43.1	MJ/kg fuel	LHV diesel (5% RME)	Gode et al. (2011)
0.85	kg/l	Density diesel	Neste Corporation (2020)
11.45	MJ/km	Fuel consumption	Calculation
225.96	kg CO_2/truck	CO_2 emissions per truck	Calculation
0.099	kg CH_4/truck	CH_4 emissions per truck	Calculation
0.0067	kg N_2O/truck	N_2O emissions per truck	Calculation
260	km	Road distance Nynäshamn – Uppsala (roundtrip)	Google maps
60	tons/truck	Size of truck	Assumption
3009059	kg LNG/d	Amount of LNG transported per day	Natural gas calculations
50.2	trucks/d	Number of trucks per day	Calculation
11332	kg CO_2/d	CO_2 emissions per day (roundtrip)	Calculation

4.97	kg CH_4/d	CH_4 emissions per day (roundtrip)	Calculation
0.33	kg N_2O/d	N_2O emissions per day (roundtrip)	Calculation

CO_2 transportation: Truck Uppsala - Gothenburg

Value	Unit	Description	Source
0.87	kg CO_2/km	CO_2 emissions/ truck-km	Calculation based on LNG truck transport
0.00038	kg CH_4/km	CH_4 emissions/ truck-km	Calculation based on LNG truck transport
0.000026	kg N_2O/km	N_2O emissions/ truck-km	Calculation based on LNG truck transport
912	km	Road distance Uppsala – Gothenburg (roundtrip)	Calculation
60	tons/truck	Size of truck	Assumption
4102320	kg CO_2/ d	Amount of CO_2 captured per day	Calculation
68	trucks/d	Number of trucks per day	Calculation
54191.93	kg CO_2/d	CO_2 emissions per day (roundtrip)	Calculation
23.77	kg CH_4/d	CH_4 emissions per day (roundtrip)	Calculation
1.60	kg N_2O/d	N_2O emissions per day (roundtrip)	Calculation

CO_2 transportation: Ship Gothenburg - Bergen

Value	Unit	Description	Source
700	nautical miles	Sea distance (roundtrip)	Sea-distances (2021)
6.7	g/MJ fuel	Bunker oil: CO_2 emissions to air WTT	Gode et al. (2011)
0.073	g/MJ fuel	Bunker oil: CH_4 emissions to air WTT	ibid
0.00015	g/MJ fuel	Bunker oil: N_2O emissions to air WTT	ibid
79	g/MJ fuel	Bunker oil: CO_2 emissions to air TTW	ibid
0.00046	g/MJ fuel	Bunker oil: CH_4 emissions to air TTW	ibid
0.0036	g/MJ fuel	Bunker oil: N_2O emission to air TTW	ibid
1993215	MJ fuel/ship	Fuel consumption per ship (roundtrip)	Calculation
170818	kg CO_2/d	CO_2 emissions per day (roundtrip)	Calculation
146	kg CH_4/d	CH_4 emissions per day (roundtrip)	Calculation
7.5	kg N_2O/d	N_2O emissions per day (roundtrip)	Calculation

Summary

In this section, all emissions from the previous sections are summarized.

Grey H2

Value	Unit	Description	Source
1174359	kg CO_2/d	CO_2 emissions from natural gas production	Natural Gas production
150162	kg CO_2/d	CO_2 emissions from LNG transport	Transportation
8340461	kg CO_2/d	CO_2 emissions from SMR process	Grey H_2
9664982	kg CO_2/d	Total CO_2 emissions per day	Calculation
11.44	kg CO_2/kg H_2	CO_2 emissions per produced kg H_2	Calculation
8850	kg CH_4/d	CH_4 emissions from natural gas production	Natural Gas production
124	kg CH_4/d	CH_4 emissions from LNG transport	Transportation
0.00	kg CH_4/d	CH_4 emissions from SMR process	Grey H_2
8974	kg CH_4/d	Total CH_4 emissions per day	Calculation
0.011	kg CH_4/kg H_2	CH_4 emissions per produced kg H_2	Calculation
40.66	kg N_2O/d	N_2O emissions from natural gas production	Natural Gas production
6.4	kg N_2O/d	N_2O emissions from LNG transport	Transportation
0.00	kg N_2O/d	N_2O emissions from SMR process	Grey H_2
47	kg N_2O/d	Total N_2O emissions per day	Calculation
0.000056	kg N_2O/kg H_2	N_2O emissions per produced kg H_2	Calculation
9946674	kg CO_2-eq/d	GWP for grey H_2 per day	Calculation
12	kg CO_2-eq/kg H_2	GWP for grey H_2 per kg H_2	Calculation

Blue H2

Value	Unit	Description	Source
1174359	kg CO_2/d	CO_2 emissions from natural gas production	Natural Gas production
150162	kg CO_2/d	CO_2 emissions of LNG transport	Transportation
4625593	kg CO_2/d	CO_2 emissions from SMR + CCS process	Blue H2
225011	kg CO_2/d	CO_2 emissions of CO_2 transport	Transportation
6175124	kg CO_2/d	Total CO_2 emissions per day	Calculation
7.3	kg CO_2/kg H_2	CO_2 emissions per produced kg H_2	Calculation
8850	kg CH_4/d	CH_4 emissions from natural gas production	Natural Gas production
124	kg CH_4/d	CH_4 emissions from LNG transport	Transportation
0.00	kg CH_4/d	CH_4 emissions from SMR + CCS process	Blue H_2
170	kg CH_4/d	CH_4 emissions of CO_2 transport	Transportation
9144	kg CH_4/d	Total CH_4 emissions per day	Calculation
0.0011	kg CH_4/kg H_2	CH_4 emissions per produced kg H_2	Calculation
41	kg N_2O/d	N_2O emissions from natural gas production	Natural Gas production
6.4	kg N_2O/d	N_2O emissions from LNG transport	Transportation
0.00	kg N_2O/d	N_2O emissions from SMR + CCS process	Blue H_2

9.1	kg N_2O/d	N_2O emissions of CO2 transpor	Transportation
47	kg N_2O/d	Total N_2O emissions per day	Calculation
0.000056	kg N_2O/kg H_2	N_2O emissions per produced kg H_2	Calculation
6443634	kg CO_2-eq/d	GWP for blue H_2 per day	Calculation
7.7	kg CO_2-eq/kg H_2	GWP for blue H_2 per kg H_2	Calculation

Beige H2

Value	Unit	Value	Source
-6926044	kg CO_2/d	CO_2 emissions from biogas production	Biogas production
8340461	kg CO_2/d	CO_2 emissions from SMR process	Beige H_2
1414416	kg CO_2/d	Total CO_2 emissions per day	Calculation
1.7	kg CO_2/kg H_2	CO_2 emissions per produced kg H_2	Calculation
38769	kg CH_4/d	CH_4 emissions from natural gas production	Biogas production
0.00	kg CH_4/d	CH_4 emissions from SMR process	Beige H_2
38769	kg CH_4/d	Total CH_4 emissions per day	Calculation
0.046	kg CH_4/kg H_2	CH_4 emissions per produced kg H_2	Calculation
0.00	kg N_2O/d	N_2O emissions from natural gas production	Biogas production
0.00	kg N_2O/d	N_2O emissions from SMR process	Beige H_2
0.00	kg N_2O/d	Total N_2O emissions per day	Calculation
0.00	kg N_2O/kg H_2	N_2O emissions per produced kg H_2	Calculation
2499957	kg CO_2-eq/d	GWP for beige H_2 per day	Calculation
3.0	kg CO_2-eq/kg H_2	GWP for beige H_2 per kg H_2	Calculation

Orange H2

Value	Unit	Value	Unit
-6926044	kg CO_2/d	CO_2 emissions from biogas production	Biogas production
4625593	kg CO_2/d	CO_2 emissions from SMR + CCS process	Orange H_2
225011	kg CO_2/d	CO_2 emissions of CO_2 transport	Transportation
-2075441	kg CO_2/d	Total CO_2 emissions per day	Calculation
-2.5	kg CO_2/kg H_2	CO_2 emissions per produced kg H_2	Calculation
38769	kg CH_4/d	CH_4 emissions from natural gas production	Biogas production
0.00	kg CH_4/d	CH_4 emissions from SMR + CCS process	Orange H_2
170	kg CH_4/d	CH_4 emissions of CO_2 transport	Transportation
38940	kg CH_4/d	Total CH_4 emissions per day	Calculation
0.046	kg CH_4/kg H_2	CH_4 emissions per produced kg H_2	Calculation
0.00	kg N_2O/d	N_2O emissions from biogas production	Biogas production
0.00	kg N_2O/d	N_2O emissions from SMR + CCS process	Orange H_2
9.1	kg N_2O/d	N_2O emissions of CO_2 transport	Transportation
9.1	kg N_2O/d	Total N_2O emissions per day	Calculation
0.000011	kg N_2O/kg H_2	N_2O emissions per produced kg H_2	Calculation

-982730	kg CO_2-eq/d	GWP for Orange H_2 per day	Calculation
-1.2	kg CO_2-eq/kg H_2	GWP for Orange H_2 per kg H2	Calculation

Green H2

Value	Unit	Value	Unit
686587	kg CO_2/d	CO_2 emissions from required electricity	Green H_2
686587	kg CO_2/d	Total CO_2 emissions per day	Calculation
0.81	kg CO_2/kg H_2	CO_2 emissions per produced kg H_2	Calculation
156	kg CH_4/d	CH_4 emissions from required electricity	Green H_2
156	kg CH_4/d	Total CH_4 emissions per day	Calculation
0.00018	kg CH_4/kg H_2	CH_4 emissions per produced kg H_2	Calculation
23	kg N_2O/d	N_2O emissions from required electricity	Green H_2
23	kg N_2O/d	Total N_2O emissions per day	Calculation
0.000027	kg N_2O/kg H_2	N_2O emissions per produced kg H_2	Calculation
697009	kg CO_2-eq/d	GWP for Green H_2 per day	Calculation
0.83	kg CO_2-eq/kg H_2	GWP for Green H_2 per kg H_2	Calculation

Fuelling and driving vehicles

In this section, data and calculations for the usage of H_2 as a fuel in heavy FC trucks are presented. A conventional IC diesel truck is used as a reference.

Heavy truck

Value	Unit	Description	Source
8.0	kg H_2/100 km	Fuel consumption heavy-duty FC truck	Assumption[18]
33.2	l/ 100 km	Fuel consumption heavy-duty diesel truck	Trafikverket (2019)
4 176 057 550	km/ year	Distance driven heavy trucks, Sweden 2019	Trafikanalys (2020a)
334 084 604	kg H_2/ year	Annual fuel consumption FC heavy trucks	Calculation
915 300	kg H_2/ day	Daily fuel consumption FC heavy trucks	Calculation
92.3	%	Share of diesel withing heavy truck sector	Trafikverket (2020a)
40 108 000 000	tonne-km/year	Traffic performance by heavy truck, 2019	Trafikanalys (2020b)
844 822	kg H_2/ day	kg H_2 to cover diesel share of heavy trucks	Calculation <- input for H2 production

Emission diesel

Value	Unit	Value	Unit
6.32	g/MJ fuel	Diesel (5% RME): CO_2 emissions to air WTT	(Gode et al. 2011)
0.0328	g/MJ fuel	Diesel (5% RME): CH_4 emissions to air WTT	ibid
0.00104	g/MJ fuel	Diesel (5% RME): N_2O emissions to air WTT	ibid
69.6	g/MJ fuel	Diesel (5% RME): CO_2 emissions to air TTW	ibid
0.000500	g/MJ fuel	Diesel (5% RME): CH_4 emissions to air TTW	ibid
0.00120	g/MJ fuel	Diesel (5% RME): N_2O emissions to air TTW	ibid
3137.7	kt CO_2/year	Diesel: CO_2 emissions heavy truck	SCB (2021)
4.1	ton CH_4/year	Diesel: CH_4 emissions heavy truck	ibid
220.2	ton N_2O/year	Diesel: N_2O emissions heavy truck	ibid
3629343009	kg CO_2/year	CO_2 emissions diesel WTW	Calculation[19]
1591901	kg CH_4/year	CH_4 emissions diesel WTW	Calculation[20]
107083	kg N_2O/year	N_2O emissions diesel WTW	Calculations[21]
3702293186	kg CO_2-eq/year	GWP for diesel emissions	Calculation

GWP for different fuels

Value	Unit	Description	Source
0.092	kg CO_2-eq/tonne-km	Diesel truck	Calculation
0.091	kg CO_2-eq/tonne-km	Grey H_2 fuel cell truck	Calculation
0.059	kg CO_2-eq/tonne-km	Blue H_2 fuel cell truck	Calculation
0.023	kg CO_2-eq/tonne-km	Beige H_2 fuel cell truck	Calculation
-0.0089	kg CO_2-eq/tonne-km	Orange H_2 fuel cell truck	Calculation
0.0063	kg CO_2-eq/tonne-km	Green H_2 fuel cell truck	Calculation

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[18] Assumption is based on data from sources FCH2 JU & Berger (2017) and Fuel Cells Works (2019)

[19] Calculations based on data from Gode et al. (2011), verified with SCB (2021)

[20] ibid

[21] ibid

Appendix II: Time dependent climate impact

In this section, calculations and simulations for the time dependent LCA are presented. These are the equations implemented in the Octave Software, as well as the relevant variables and coefficients.

Absolute Temperature Change Potential (AGTP)

The following equations express the absolute global temperature change potential (AGTP) of the greenhouse gases CO_2, CH_4 and N_2O. The following equations were calculated in Octave Software, in a script by Ericsson (2014). The AGTPs for CO_2, CH_4 and N_2O were expressed in [K/kg] and calculated through equations 25, 26 and 27 (Collins et al. 2013).

$$AGTP^{CO2}(t) = RE^{CO2}\sum_{j=1}^{2}\left\{a_0 c_j\left(1-e^{-\frac{t}{d_j}}\right)+\sum_{i=1}^{3}\frac{a_i\alpha_i^{CO_2}c_j}{\alpha_i^{CO_2}-d_j}\left(e^{-\frac{t}{\alpha_i^{CO_2}}}-e^{-\frac{t}{d_j}}\right)\right\} \quad (25)$$

$$AGTP^{CH}\ (t) = RE^{CH4}\sum_{j=1}^{2}\left\{\frac{\alpha^{CH_4}c_j}{\alpha^{CH_4}-d_j}\left(e^{-\frac{t}{\alpha^{CH_4}}}-e^{-\frac{t}{d_j}}\right)\right\} \quad (26)$$

$$AGTP^{N2O}(t) = RE^{N2O}\sum_{j=1}^{2}\left\{\frac{\alpha^{N_2O}c_j}{\alpha^{N_2O}-d_j}\left(e^{-\frac{t}{\alpha^{N_2O}}}-e^{-\frac{t}{d_j}}\right)\right\} \quad (27)$$

Coefficients of c_j and d_j are parameters of the impulse response functions (Boucher & Reddy 2008). Coefficients of $a_{0\text{-}3}$ are unitless and α_{1-3}^{CO2}, α^{CH4} and α^{N2O} represent the emission response timescales in years (Collins et al. 2013). Response coefficients are shown in table 4.

Table 5. Response coefficients

parameter	j, i = 0	j, i = 1	j, i = 2	j, i = 3	unit	source
a_i	0.2173	0.2240	0.2824	0.2763	-	(IPCC 2013)
c_j	-	0.631	0.429	-	K/Wm^2	(Boucher & Reddy 2008)
d_j	-	8.4	409.5	-	years	(Boucher & Reddy 2008)
α_{1-3}^{CO2}	-	394.4	36.54	4.304	years	(IPCC 2013)
α^{CH4}	-	12.4	12.4	-	years	(IPCC 2013)
α^{N2O}	-	121.0	121.0	-	years	(IPCC 2013:2)

The time horizon is expressed as a vector t, representing the evaluated time interval which is 100 years for this study. The radiative efficiencies of CO_2, CH_4 and N_2O respectively, are expressed as RE^{CO2}, RE^{CH4} and RE^{N2O}, equations 28, 29 and 30 (Ericsson 2014).

$$RE^{CO2} = \frac{\Delta F^{CO2}}{f_{CO}} \quad [W/m^2kg] \tag{28}$$

$$RE^{CH4} = \Delta F^{CH4} \cdot \frac{1+f_1+f_2}{f_{CH_4}} \quad [W/m^2kg] \tag{29}$$

$$RE^{N2O} = \frac{\Delta F^{N2O}}{f_{N2O}} \quad [W/m^2kg] \tag{30}$$

Methane affects the ozone and stratospheric water, which is expressed in parameters of f_1 and f_2, table 5. ΔF^{CO2}, ΔF^{CH4} and ΔF^{N2O} are the emission volumes of CO_2, CH_4 and N_2O respectively, expressed in equations 31, 32 and 33 (IPCC 2001).

$$\Delta F^{CO2} = \alpha_C \cdot \ln \frac{C}{C_0} \quad [W/m^2] \tag{31}$$

$$\Delta F^{CH4} = \alpha_m \cdot \left(\sqrt{M} - \sqrt{M_0}\right) - \left(f(M, N_0) - f(M_0, N_0)\right) \quad [W/m^2] \tag{32}$$

$$\Delta F^{N2O} = \alpha_n \cdot \left(\sqrt{N} - \sqrt{N_0}\right) - \left(f(M_0, N) - f(M_0, N_0)\right) \quad [W/m^2] \tag{33}$$

Following function (34) represents the function of CH_4 and N_2O concentrations (IPCC 2001), and values from table 5 are used.

$$f(M, N) = 0.47 \cdot \ln\left[1 + 2.01 \cdot 10^{-5}(MN)^{0.75} + 5.31 \cdot 10^{-15} M (MN)^{1.52}\right] \tag{34}$$

To convert volume to kg gas, the following help functions are needed for f_{CO2}, f_{CH4} and f_{N2O} respectively, equations 35, 36 and 37 (Ericsson 2014), with values from table 5.

$$f_{CO} = \frac{T_m/1000000}{M_{air} \cdot M_{CO} \cdot (C - C_0)} \tag{35}$$

$$f_{CH4} = \frac{T_m/1000000}{M_{air} \cdot M_{CH} \cdot (M - M_0)} \tag{36}$$

$$f_{N2O} = \frac{T_m/1000000}{M_{air} \cdot M_{N2O} \cdot (N - N_0)} \tag{37}$$

Table 6. Parameters for time-dependent calculations.

parameter	value	unit	description	source
f_1	0.5	-	CH_4 effect on ozone	(IPCC 2013)
f_2	0.15	-	CH_4 effect on stratospheric water	(IPCC 2013)
C_0	391	ppm	CO_2 concentration	(IPCC 2013)
C	392	ppm	New CO_2 concentration	(IPCC 2013)
M_0	1803	ppb	CH_4 concentration	(IPCC 2013)
M	1804	ppb	New CH_4 concentration	(IPCC 2013)
N_0	324	ppb	N_2O concentration	(IPCC 2013:2)
N	325	ppb	New N_2O concentration	(IPCC 2013)
α_c	5.35	unitless	Constant for CO_2	(IPCC 2001)
α_m	0.036	unitless	Constant for CH_4	(IPCC 2001)
α_n	0.12	unitless	Constant for N_2O	(IPCC 2001:20)
M_{CO2}	44.0098	g/mol	Molecular weight of CO_2	
M_{CH4}	16.0428	g/mol	Molecular weight of CH_4	
M_{N2O}	44.0129	g/mol	Molecular weight of N_2O	
M_{air}	28.97	g/mol	Molecular weight of air	
T_m	$5.1352 \cdot 10^{18}$	kg	Mean dry mass value of atmosphere	(Trenberth & Smith 2005)

Appendix III: Future scenarios

Emission vectors for the reference scenario, scenario 1, scenario 2, scenario 3, extreme 1 and extreme 2 are demonstrated in this section. For the reference scenario, only diesel fuel with 5% RME is used to cover the diesel share of the domestic heavy truck transport.

Reference scenario

Year	kg CO_2/tonne-km	kg CH_4/tonne-km	kg N_2O/tonne-km	Diesel share
2020	0.090	0.000040	0.0000027	100%
2021	0.090	0.000040	0.0000027	100%
2022	0.090	0.000040	0.0000027	100%
2023	0.090	0.000040	0.0000027	100%
2024	0.090	0.000040	0.0000027	100%
2025	0.090	0.000040	0.0000027	100%
2026	0.090	0.000040	0.0000027	100%
2027	0.090	0.000040	0.0000027	100%
2028	0.090	0.000040	0.0000027	100%
2029	0.090	0.000040	0.0000027	100%
2030	0.090	0.000040	0.0000027	100%
2031	0.090	0.000040	0.0000027	100%
2032	0.090	0.000040	0.0000027	100%
2033	0.090	0.000040	0.0000027	100%
2034	0.090	0.000040	0.0000027	100%
2035	0.090	0.000040	0.0000027	100%
2036	0.090	0.000040	0.0000027	100%
2037	0.090	0.000040	0.0000027	100%
2038	0.090	0.000040	0.0000027	100%
2039	0.090	0.000040	0.0000027	100%
2040	0.090	0.000040	0.0000027	100%
2041	0.090	0.000040	0.0000027	100%
2042	0.090	0.000040	0.0000027	100%
2043	0.090	0.000040	0.0000027	100%
2044	0.090	0.000040	0.0000027	100%
2045	0.090	0.000040	0.0000027	100%
2046	0.090	0.000040	0.0000027	100%
2047	0.090	0.000040	0.0000027	100%
2048	0.090	0.000040	0.0000027	100%
2049	0.090	0.000040	0.0000027	100%
2050	0.090	0.000040	0.0000027	100%

Scenario 1

Year	**kg CO_2/tonne-km**	**kg CH_4/tonne-km**	**kg N_2O/tonne-km**	**Grey H_2**	**Blue H_2**
2020	0.090	0.000040	0.0000027	100%	0%
2021	0.090	0.000040	0.0000027	100%	0%
2022	0.090	0.000040	0.0000026	100%	0%
2023	0.090	0.000041	0.0000026	90%	10%
2024	0.090	0.000041	0.0000026	80%	20%
2025	0.090	0.000042	0.0000026	70%	30%
2026	0.090	0.000042	0.0000026	60%	40%
2027	0.089	0.000042	0.0000025	50%	50%
2028	0.089	0.000043	0.0000025	40%	60%
2029	0.089	0.000043	0.0000025	30%	70%
2030	0.088	0.000043	0.0000025	20%	80%
2031	0.088	0.000044	0.0000025	10%	90%
2032	0.087	0.000044	0.0000024	0%	100%
2033	0.086	0.000045	0.0000024	0%	100%
2034	0.086	0.000046	0.0000024	0%	100%
2035	0.085	0.000046	0.0000023	0%	100%
2036	0.085	0.000047	0.0000023	0%	100%
2037	0.084	0.000048	0.0000022	0%	100%
2038	0.083	0.000049	0.0000022	0%	100%
2039	0.082	0.000050	0.0000021	0%	100%
2040	0.081	0.000051	0.0000021	0%	100%
2041	0.080	0.000053	0.0000020	0%	100%
2042	0.079	0.000054	0.0000019	0%	100%
2043	0.078	0.000056	0.0000018	0%	100%
2044	0.076	0.000058	0.0000017	0%	100%
2045	0.074	0.000060	0.0000016	0%	100%
2046	0.073	0.000062	0.0000015	0%	100%
2047	0.070	0.000065	0.0000014	0%	100%
2048	0.068	0.000068	0.0000012	0%	100%
2049	0.065	0.000072	0.0000010	0%	100%
2050	0.062	0.000075	0.00000083	0%	100%

Scenario 2

Year	kg CO_2/tonne-km	kg CH_4/tonne-km	kg N_2O/tonne-km	Grey	Blue	Beige	Orange
2020	0.090	0.000040	0.0000027	90%	0%	10%	0%
2021	0.090	0.000040	0.0000027	90%	0%	10%	0%
2022	0.090	0.000041	0.0000026	90%	0%	10%	0%
2023	0.090	0.000041	0.0000026	80%	10%	5%	5%
2024	0.090	0.000042	0.0000026	60%	30%	5%	5%
2025	0.089	0.000043	0.0000026	20%	70%	5%	5%
2026	0.088	0.000043	0.0000026	0%	90%	0%	10%
2027	0.088	0.000044	0.0000025	0%	90%	0%	10%
2028	0.088	0.000045	0.0000025	0%	90%	0%	10%
2029	0.087	0.000045	0.0000025	0%	90%	0%	10%
2030	0.087	0.000046	0.0000025	0%	90%	0%	10%
2031	0.086	0.000046	0.0000025	0%	90%	0%	10%
2032	0.086	0.000047	0.0000024	0%	90%	0%	10%
2033	0.085	0.000048	0.0000024	0%	90%	0%	10%
2034	0.085	0.000049	0.0000024	0%	90%	0%	10%
2035	0.084	0.000050	0.0000023	0%	90%	0%	10%
2036	0.083	0.000052	0.0000023	0%	90%	0%	10%
2037	0.083	0.000053	0.0000022	0%	90%	0%	10%
2038	0.082	0.000055	0.0000022	0%	90%	0%	10%
2039	0.081	0.000056	0.0000021	0%	90%	0%	10%
2040	0.079	0.000058	0.0000021	0%	90%	0%	10%
2041	0.078	0.000061	0.0000020	0%	90%	0%	10%
2042	0.077	0.000063	0.0000019	0%	90%	0%	10%
2043	0.075	0.000066	0.0000018	0%	90%	0%	10%
2044	0.073	0.000069	0.0000017	0%	90%	0%	10%
2045	0.071	0.000073	0.0000016	0%	90%	0%	10%
2046	0.069	0.000077	0.0000015	0%	90%	0%	10%
2047	0.066	0.000081	0.0000013	0%	90%	0%	10%
2048	0.063	0.000086	0.0000012	0%	90%	0%	10%
2049	0.060	0.000092	0.0000010	0%	90%	0%	10%
2050	0.056	0.000098	0.00000080	0%	90%	0%	10%

Scenario 3

Year	**kg CO$_2$/tonne-km**	**kg CH$_4$/tonne-km**	**kg N$_2$O/tonne-km**	**Grey**	**Blue**	**Beige**	**Orange**	**Green**
2020	0.090	0.000040	0.0000027	90%	0%	10%	0%	0%
2021	0.090	0.000040	0.0000027	90%	0%	10%	0%	0%
2022	0.090	0.000041	0.0000026	90%	0%	10%	0%	0%
2023	0.090	0.000041	0.0000026	75%	10%	5%	5%	5%
2024	0.090	0.000042	0.0000026	55%	30%	5%	5%	5%
2025	0.089	0.000043	0.0000026	15%	70%	5%	5%	5%
2026	0.088	0.000043	0.0000026	0%	80%	0%	10%	10%
2027	0.088	0.000043	0.0000025	0%	75%	0%	10%	15%
2028	0.087	0.000043	0.0000025	0%	70%	0%	10%	20%
2029	0.086	0.000043	0.0000025	0%	60%	0%	10%	30%
2030	0.085	0.000043	0.0000025	0%	50%	0%	10%	40%
2031	0.084	0.000043	0.0000024	0%	48%	0%	10%	42%
2032	0.084	0.000043	0.0000024	0%	46%	0%	10%	44%
2033	0.083	0.000044	0.0000024	0%	44%	0%	10%	46%
2034	0.082	0.000044	0.0000023	0%	42%	0%	10%	48%
2035	0.080	0.000044	0.0000023	0%	40%	0%	10%	50%
2036	0.079	0.000044	0.0000022	0%	38%	0%	10%	52%
2037	0.078	0.000045	0.0000022	0%	36%	0%	10%	54%
2038	0.076	0.000045	0.0000021	0%	34%	0%	10%	56%
2039	0.074	0.000045	0.0000021	0%	32%	0%	10%	58%
2040	0.071	0.000045	0.0000020	0%	30%	0%	10%	60%
2041	0.068	0.000045	0.0000019	0%	25%	0%	10%	65%
2042	0.065	0.000044	0.0000018	0%	20%	0%	10%	70%
2043	0.061	0.000043	0.0000017	0%	15%	0%	10%	75%
2044	0.055	0.000040	0.0000016	0%	5%	0%	10%	85%
2045	0.050	0.000038	0.0000014	0%	0%	0%	10%	90%
2046	0.045	0.000037	0.0000013	0%	0%	0%	10%	90%
2047	0.040	0.000037	0.0000011	0%	0%	0%	10%	90%
2048	0.034	0.000037	0.00000092	0%	0%	0%	10%	90%
2049	0.027	0.000037	0.00000071	0%	0%	0%	10%	90%
2050	0.019	0.000036	0.00000048	0%	0%	0%	10%	90%

Extreme scenario 1

Year	**kg CO_2/tonne-km**	**kg CH_4/tonne-km**	**kg N_2O/tonne-km**	**Grey H_2**
2020	0.090	0.000040	0.0000027	100%
2021	0.090	0.000040	0.0000027	100%
2022	0.090	0.000040	0.0000026	100%
2023	0.090	0.000041	0.0000026	100%
2024	0.090	0.000041	0.0000026	100%
2025	0.090	0.000041	0.0000026	100%
2026	0.090	0.000042	0.0000026	100%
2027	0.090	0.000042	0.0000025	100%
2028	0.090	0.000043	0.0000025	100%
2029	0.090	0.000043	0.0000025	100%
2030	0.090	0.000043	0.0000025	100%
2031	0.090	0.000044	0.0000025	100%
2032	0.090	0.000044	0.0000024	100%
2033	0.090	0.000045	0.0000024	100%
2034	0.090	0.000045	0.0000024	100%
2035	0.090	0.000046	0.0000023	100%
2036	0.090	0.000047	0.0000023	100%
2037	0.090	0.000048	0.0000022	100%
2038	0.090	0.000049	0.0000022	100%
2039	0.090	0.000050	0.0000021	100%
2040	0.090	0.000051	0.0000021	100%
2041	0.090	0.000052	0.0000020	100%
2042	0.090	0.000054	0.0000019	100%
2043	0.090	0.000055	0.0000018	100%
2044	0.089	0.000057	0.0000017	100%
2045	0.089	0.000059	0.0000016	100%
2046	0.089	0.000062	0.0000015	100%
2047	0.089	0.000064	0.0000014	100%
2048	0.089	0.000067	0.0000012	100%
2049	0.089	0.000071	0.0000010	100%
2050	0.088	0.000074	0.00000083	100%

Extreme scenario 2

Year	kg CO_2/tonne-km	kg CH_4/tonne-km	kg N_2O/tonne-km	Orange H_2
2020	0.090	0.000040	0.0000027	100%
2021	0.090	0.000042	0.0000026	100%
2022	0.089	0.000045	0.0000026	100%
2023	0.088	0.000048	0.0000026	100%
2024	0.087	0.000050	0.0000026	100%
2025	0.086	0.000053	0.0000026	100%
2026	0.085	0.000056	0.0000025	100%
2027	0.084	0.000058	0.0000025	100%
2028	0.083	0.000061	0.0000025	100%
2029	0.082	0.000064	0.0000025	100%
2030	0.081	0.000067	0.0000024	100%
2031	0.080	0.000070	0.0000024	100%
2032	0.079	0.000073	0.0000024	100%
2033	0.077	0.000077	0.0000024	100%
2034	0.076	0.000082	0.0000023	100%
2035	0.074	0.000087	0.0000023	100%
2036	0.072	0.000093	0.0000022	100%
2037	0.070	0.000099	0.0000022	100%
2038	0.067	0.00011	0.0000021	100%
2039	0.065	0.00011	0.0000021	100%
2040	0.062	0.00012	0.0000020	100%
2041	0.058	0.00013	0.0000019	100%
2042	0.054	0.00014	0.0000018	100%
2043	0.050	0.00016	0.0000017	100%
2044	0.045	0.00017	0.0000016	100%
2045	0.039	0.00019	0.0000015	100%
2046	0.033	0.00020	0.0000013	100%
2047	0.026	0.00022	0.0000012	100%
2048	0.019	0.00025	0.0000010	100%
2049	0.010	0.00027	0.00000077	100%
2050	0.00051	0.00030	0.00000054	100%

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