

Life cycle and techno-economic assessment of Power-to-Gas processes in Germany

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Danksagung

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Abstract

Aufgrund des voranschreitenden Klimawandels wird Deutschlands Energiesystem zunehmend auf erneuerbare Energien umgestellt, was zu neuen Herausforderungen führt, z. B. im Winter, wenn weniger Wind- und Solarenergie zugänglich sind. In diesem Zusammenhang ist zu erwarten, dass die Nachfrage nicht ausreichend gedeckt werden kann. Um diesem Problem zu begegnen, bieten sich Power-to-Gas Anlagen als langfristige Speicherlösung von erneuerbaren Energien an, da das Erdgasnetz als langfristiger Speicher bereits vorhanden ist, sodass Investitionskosten reduziert und große Mengen an Energie gespeichert werden können. Aufgrund des Potenzials von Power-to-Gas als Speicherlösung für die Energiewende in Deutschland und des zunehmenden Interesses an Themen wie Nachhaltigkeit in der Gesellschaft zielt diese Dissertation darauf ab, herauszufinden, welche potenziellen Umweltauswirkungen und Gestehungs- und Umweltkosten bei der Erzeugung von Wasserstoff und Synthetic Natural Gas in Power-to-Gas Prozessen entstehen. Dazu sind verschiedene Elektrolysetechnologien, CO₂-Quellen und Energieszenarien berücksichtigt worden. Die Forschungsarbeit kommt zu den Ergebnissen, dass Power-to-Gas Prozesse mit Festoxid-Elektrolysezellen (2019, 2030) und Polymer-Elektrolyt-Membran Elektrolyse (2050, erneuerbare Energien) die umweltfreundlichsten sind. Darüber hinaus verursachen nur die aus 100 % erneuerbaren Energien hergestellten Gase weniger Treibhausgasemissionen als die berücksichtigten konventionellen Energiequellen und Kraftstoffe, unter der Annahme, dass diese wieder in elektrische Energie umgewandelt werden oder als Kraftstoff für Autos zum Einsatz kommen. Bezüglich der Gestehungskosten von Wasserstoff und Synthetic Natural Gas resultieren höhere Werte im Vergleich zu Peer-Studien, da nach der Methode von Rubin et al. mehr Kostenfaktoren berücksichtigt werden. Die Berechnung der Umweltkosten bietet eine Basis, um nachhaltige Prozesse zu fördern. Die Arbeit bietet außerdem eine Grundlage für weitere Forschungsarbeiten. So könnten mit den erstellten Lebenszyklusmodellen potenzielle Umweltauswirkungen von Power-to-Gas Prozessen in anderen Ländern modelliert werden. Außerdem könnten hinsichtlich der Gestehungskosten zukünftige Werte für z. B. 2030 oder 2050 ermittelt werden.

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Abkürzungsverzeichnis

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AEL	Alkalische Elektrolyse
BEC	Bare Erected Cost
CAPEX	Capital Expenditures
CNG	Compressed Natural Gas
ct	Cent
DVGW	Deutscher Verein des Gas- und Wasserfaches e.V.
EE	Erneuerbare Energien
EU	Europäische Union
GW	Gigawatt
GWP	Global Warming Potential
ILCD	International Life Cycle Data system
IPCC	Intergovernmental Panel on Climate Change
ISO	Internationale Organisation für Normung
kg	Kilogramm
km	Kilometer
kWh	Kilowattstunde
LCA	Life-Cycle Assessment
MW	Megawatt
MWh	Megawattstunde
NG	Natural Gas
PEM	Polymer-Elektrolyt-Membran-Elektrolysezelle
PtG	Power-to-Gas
PtH	Power-to-Hydrogen
PtM	Power-to-Methane
ReCiPe	Methode, um Umweltauswirkungen zu berechnen
SNG	Synthetic Natural Gas
SOEC	Festoxid-Elektrolyse-Zellen
TOC	Total Overnight Cost
TWh	Terawattstunde

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1 Einleitung

Die nachfolgende Einleitung setzt sich aus der Relevanz und Motivation sowie aus der Zielsetzung und dem Aufbau der Arbeit zusammen.

1.1 Relevanz und Motivation der Arbeit

Aufgrund des voranschreitenden Klimawandels und des Pariser Abkommens, die globale Erwärmung auf weniger als 2 Grad Celsius im Vergleich zum vorindustriellen Zeitraum zu begrenzen, hat die Bundesregierung beschlossen, die CO₂-Emissionen bis 2040 um 88 % gegenüber dem Basisjahr 1990 zu reduzieren [1,2]. Um dieses Ziel zu erreichen, ist der Ausbau der Wind- und Solarenergieanlagen ein zentraler Bestandteil der deutschen Energiewende. So soll, nach einem von Agora Energiewende entworfenen Szenario, die installierte Leistung bis 2030 gegenüber dem Jahr 2020 um etwa 83 GW steigen, was einem Anstieg von mehr als zwei Dritteln bedeutet [3]. Allerdings bringt der Ausbau der erneuerbaren Energien neue Herausforderungen mit sich, da Wind- und Solarenergie nicht immer zur Verfügung stehen. Was passiert zum Beispiel im Winter, wenn kaum Wind- und Solarenergie verfügbar sind? Wie kann die Nachfrage in dieser Jahreszeit befriedigt werden? Laut dem Deutschen Vereins des Gas- und Wasserfaches (DVGW) besteht die größte Herausforderung darin, Angebot und Nachfrage für elektrische Energie in dieser Jahreszeit in Einklang zu bringen [4]. In diesem Zusammenhang wird eine geschätzte Menge von 35 TWh als langfristige Reserve für die Wintermonate benötigt, um einen Blackout zu vermeiden [5,6]. Diesbezüglich bietet Power-to-Gas (PtG) als Langzeitspeicherlösung ein großes Potenzial, um die geschätzte Menge von 35 TWh als Reserve bereitzustellen und Blackouts während der Wintermonate zu vermeiden [7,8,9], da die Erdgasnetzinfrastruktur in Deutschland mit einer Länge von ca. 500.000 km und einer Speicherkapazität von rund 350 TWh bereits vorhanden ist [5]. Auch der DVGW sieht PtG als alternativlos an und damit als einzige Technologie für die saisonale Speicherung von Energie in großen Mengen [10]. Daher kann PtG aufgrund der bereits vorhandenen Erdgasnetzinfrastruktur als zukünftige Langzeitspeicherlösung eine essenzielle Rolle in der Energiewende spielen.

1.2 Zielsetzung und Aufbau der Arbeit

Aufgrund des vielversprechenden Potenzials als langfristige Speicherlösung besteht ein erhebliches Interesse an PtG-Lösungen von verschiedenen

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Interessengruppen, um eine sichere Versorgung mit elektrischer Energie in den Wintermonaten zu gewährleisten [4,11]. Darüber hinaus nimmt die Fokussierung auf das Thema Klimawandel in der deutschen Gesellschaft (u. a. Fridays for Future) weiterhin zu, sodass Themen wie Nachhaltigkeit weiter in den Vordergrund und das Bewusstsein der Menschen rücken [12]. Aus diesen Gründen beschäftigt sich diese Arbeit mit der Lebenszyklus- und techno-ökonomischen Analyse von PtG-Prozessen, um sowohl die ökologische als auch ökonomische Seite von PtG-Prozessen zu bewerten, da nicht nur ökonomische sondern auch ökologische Aspekte eine wichtige Rolle spielen. Insgesamt besteht das übergeordnete Ziel dieser als kumulativen Dissertation eingereichten Forschungsarbeit darin, herauszufinden, welche potenziellen Umweltauswirkungen und Gestehungs- und Umweltkosten bei der Erzeugung von Wasserstoff und Synthetic Natural Gas (SNG) in PtG-Prozessen in Deutschland entstehen. Dazu sind verschiedene Elektrolysetechnologien –Alkalische Elektrolyse (AEL), Polymer-Elektrolyt-Membran Elektrolyse (PEM) und Festoxid-Elektrolysezellen (SOEC)– und CO₂-Quellen (Luft, Biomasse und Zementherstellung) für die Herstellung von Wasserstoff bzw. SNG berücksichtigt worden. Außerdem sind unterschiedliche Energieszenarien (2019, 2030, 2050, und EE (erneuerbare Energien)) mit steigendem Anteil von Wind- und Solarenergie für eine nachhaltigere Produktion berücksichtigt worden.

Das Thema ist insbesondere auch vor dem Hintergrund attraktiv, da die Bundesregierung eine Wasserstoffstrategie initiiert hat und Deutschland bis 2030 weltweit eine führende Rolle in der Wasserstoffwirtschaft einnehmen möchte, sodass grüner Wasserstoff (Power-to-Hydrogen, PtH) in Zukunft eine wesentliche Rolle spielen wird [13]. Daher bietet die Arbeit ein erhebliches Potenzial für verschiedene Interessengruppen, da nicht nur die Gestehungs- und Umweltkosten von Wasserstoff und SNG ermittelt werden, sondern auch die potenziellen Umweltauswirkungen der Herstellungsprozesse, die in Zeiten des Klimawandels von wesentlichem Interesse sind [14]. Die Ergebnisse sind daher sowohl für Forschungseinrichtungen als auch für Entscheidungsträger in Unternehmen und Politik von Interesse, vor dem Hintergrund der Energiewende, des Klimawandels und des Aufbaus der Wasserstoffwirtschaft in Deutschland und Europa.

1. Einleitung

Die Arbeit gliedert sich in zwei Teilbereiche. Zum einen der Umweltbereich, in dem die potenziellen Umweltauswirkungen der PtG-Prozesse analysiert werden, mit den folgenden Publikationen:

1. *Comparative Life-Cycle-Assessment analysis of three major water electrolysis technologies while applying various energy scenarios for a greener hydrogen production.*

(publiziert in: Journal of Energy Storage,

<https://doi.org/10.1016/j.est.2021.102759>)

2. *Comparative Life-Cycle Assessment Analysis of Power-to-Methane Plants Including Different Water Electrolysis Technologies and CO₂ Sources While Applying Various Energy Scenarios.*

(publiziert in: ACS Sustainable Chemistry & Engineering,

<https://doi.org/10.1021/acssuschemeng.1c02002>)

Zum anderen der Kostenbereich, in dem die Gestehungs- und Umweltkosten der PtG-Prozesse analysiert werden, mit folgendem publizierten Artikel.

3. *Levelized and environmental costs of power-to-gas generation in Germany.*

(publiziert in: International Journal of Hydrogen Energy,

<https://doi.org/10.1016/j.ijhydene.2023.01.347>)

Da der Verfasser für alle Artikel der alleinige Autor ist, ist eine Erklärung über den geleisteten Eigenanteil nicht notwendig.

Im Umweltteil ist eine vergleichende Lebenszyklusanalyse von verschiedenen PtG-Prozessen für die Wasserstoff- und SNG-Herstellung durchgeführt worden, für die die potenziellen Umweltauswirkungen von insgesamt acht Wirkungsindikatoren berücksichtigt worden sind (s. Abschnitt 4.1). Dazu sind, wie oben bereits erwähnt, die drei wichtigsten Wasserelektrolysetechnologien, verschiedene CO₂-Quellen und verschiedene Energieszenarien für eine nachhaltigere Produktion berücksichtigt worden. Darüber hinaus werden die Ergebnisse des Global Warming Potentials (GWP) der hergestellten Gase im Vergleich zu den Ergebnissen anderer Studien und Prozesse eingeordnet. Des Weiteren werden diese Ergebnisse mit den CO₂-Emissionen konventioneller Energiequellen und Kraftstoffe verglichen, unter der Annahme, dass die hergestellten Gase wieder zur Umwandlung in elektrische Energie und als Kraftstoff für Autos eingesetzt werden.

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Im Kostenteil werden die Gestehungs- und Umweltkosten von Wasserstoff und SNG analysiert. Dazu ist die Methode von Rubin et al. für die Berechnung der Gestehungskosten von Wasserstoff und SNG angewendet worden. Diese Methode ist im Vergleich zu anderen Methoden detaillierter [15-31]. So ist diese Methode nach Kenntnisstand des Autors noch nie für die Berechnung der Gestehungskosten für Wasserstoff und SNG in Deutschland unter Berücksichtigung der drei wichtigsten Wasserelektrolysetechnologien in einer Studie angewendet worden. Daher bietet die Studie eine neue Perspektive auf die Gestehungskosten von Wasserstoff und SNG in Deutschland. Darüber hinaus sind im dritten Artikel Umweltkosten berechnet worden, da Umweltaspekte bei der Erzeugung von Produkten immer wichtiger werden [32-34].

Aufgrund der Daten- und Informationslage konnten mit der Methode von Rubin et al. nur gegenwärtige und keine zukünftigen Werte für z. B. 2030 oder 2050 berechnet werden. In diesem Zusammenhang hat der Autor zwei weitere Forschungsbeiträge zum Thema Gestehungskosten von Wasserstoff und SNG eingereicht, die auch zukünftige Werte umfassen und über die Ergebnisse dieser Arbeit hinausgehen. Während der 4. Artikel publiziert wurde (s. u.), befindet sich der 5. Artikel noch „*under review*“.

4. *Economic analysis of synthetic natural gas production in Germany, considering different Power-to-Methane plants.* (Sustainable Energy & Fuels)
5. *Economic analysis of hydrogen production in Germany with a focus on green hydrogen, considering all three major water electrolysis technologies.* (Under Review)

Da die Ergebnisse nicht Thema dieser Arbeit sind, soll im weiteren Verlauf der Zusammenfassung nur kurz darauf eingegangen werden.

Im nachfolgenden Abschnitt werden auf Begriffsdefinitionen und Hintergründe der Arbeit eingegangen.

2 Begriffsdefinitionen und Hintergründe

In diesem Abschnitt wird darauf eingegangen, was PtG ist, welche besondere Rolle grüner Wasserstoff in der zukünftigen Energieversorgung spielen wird und warum Lebenszyklusanalysen so wichtig sind. Außerdem werden die Begriffe Gesteigungs- und Umweltkosten sowie GWP-Ergebnisse thematisiert.

2.1 Was ist PtG?

Unter PtG versteht man die Umwandlung von elektrischer Energie in ein brennbares Gas, hauptsächlich die Umwandlung von elektrischer Energie in Wasserstoff durch Wasserelektrolyse (PtH), der in das Erdgasnetz eingespeist werden kann (zulässiger volumetrischer Anteil für H₂ im Bereich von 1 % bis max. 10 %) [35,36]. Der erzeugte Wasserstoff kann mit Kohlendioxid zu SNG weiterreagieren, dessen Hauptbestandteil Methan ist (Power-to-Methane, PtM). Somit kann das produzierte SNG nach Entwässerung und Konditionierung auch in das Erdgasnetz eingespeist werden, da sich die Eigenschaften von SNG und Erdgas (NG) kaum unterscheiden [37,38]. Wie eingangs erwähnt, verfügt die Erdgasnetzinfrastruktur über eine Gesamtlänge von etwa 500.000 km und einer Speicherkapazität von etwa 350 TWh, sodass die PtG-Technologie aufgrund dieser Infrastruktur ein wichtiger Baustein der Energiewende werden kann, um zukünftig große Mengen an Energie saisonal zu speichern.

2.2 Besondere Rolle von grünem Wasserstoff

Einer besonderen Rolle für die Energiewende und das Erreichen der Pariser Klimaziele spielt grüner Wasserstoff, welcher aus erneuerbaren Energien hergestellt wird. Der Grund ist, dass mithilfe des grünen Wasserstoffs große Treibhausgasverursacher vor allem in der Industrie ersetzt werden können, wie z. B. in der Chemie- und Stahlindustrie. So können z. B. Kohle und Erdgas durch grünen Wasserstoff ersetzt werden, wodurch sich die Klimabilanz erheblich verbessern würde [13]. Gerade die Stahlindustrie trägt mit etwa 7 % der weltweiten CO₂-Emissionen signifikant zu den Treibhausgasemissionen bei, sodass sich hier unter Einsatz von grünem Wasserstoff ein erhebliches Einsparpotenzial ergibt [39,40]. Darüber hinaus kann der erzeugte grüne Wasserstoff zusammen mit CO₂ zu anderen klimafreundlichen Kraftstoffen reagieren (u. a. SNG), die ebenfalls zur Minderung der Treibhausgasemissionen eingesetzt werden können. Insgesamt ergeben sich eine Vielzahl von Einsatzmöglichkeiten für grünen Wasserstoff, weshalb die Bundesregierung mit

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der Initiierung der Wasserstoffstrategie 2020 die besondere Bedeutung dieses nachhaltigen Gases für die Energiewende und die Erreichung der Pariser Klimaschutzziele unterstrichen hat [13]. Darüber hinaus gibt es Kooperationen der Bundesregierung mit Ländern im westlichen und südlichen Afrika sowie mit Australien, da hier die Erzeugungskosten aufgrund der besseren Bedingungen für Wind- und Solarenergie (Kapazitätsfaktoren) wesentlich geringer sind [41]. Die Aussichten für grünen Wasserstoff sind also günstig, um eine besondere Rolle in der Energiewende zu spielen. Jedoch wird erst 2030 mit grünem Wasserstoff als wettbewerbsfähigen Kraftstoff gerechnet [13].

2.3 Lebenszyklusanalyse und warum sie so wichtig ist?

In Zeiten des Klimawandels spielt Nachhaltigkeit eine immer bedeutendere Rolle, um weniger Ressourcen zu verbrauchen und die Umwelt nachhaltig zu schonen. Ein wichtiges Tool für die Bewertung von Nachhaltigkeit ist die Lebenszyklusanalyse. Mithilfe der Lebenszyklusanalyse können Umweltauswirkungen von Produkten und Dienstleistungen über den gesamten Lebenszyklus (von der Wiege bis zur Bahre) analysiert und bewertet werden. Dies bietet die Möglichkeit, anhand der gewonnen Umweltinformationen, z. B. Optimierungspotenziale zu identifizieren, die dazu beitragen, die Emissionen und Umweltbelastung zu reduzieren, sodass nachhaltige Produkte geschaffen werden können. Daher trägt die Lebenszyklusanalyse zu einer nachhaltigen Gesellschaft bei [42].

Der Lebenszyklus von der Wiege bis zur Bahre, der in dieser Arbeit angewendet wurde, umfasst insgesamt fünf Phasen (Rohstoffgewinnung, Herstellung, Distribution, Nutzung und Entsorgung). Um nun die Umweltauswirkungen eines Produktes zu ermitteln, werden die gesammelten Daten (Energie- und Stoffströme) den einzelnen Phasen in Form von Prozessen zugeordnet. So werden z. B. für die Herstellung von 1 kg Wasserstoff 51 kWh elektrische Energie benötigt. Um diesen Energiestrom mit der *Life Cycle Assessment* (LCA) Software Umberto+ abzubilden, wird aus der Ecoinvent-Datenbank z. B. der Prozess Solarenergie ausgewählt und der Phase Nutzung zugeordnet. Dies wird für alle Energie- und Stoffstromflüsse entsprechend durchgeführt, sodass sich ein Fließbild des gesamten PtG-Prozesses ergibt. Anschließend werden die potenziellen Umweltauswirkungen der ausgewählten Indikatoren (s. Tab. 1) simuliert. Die Berechnung erfolgt, indem die quantitative Menge der Energie- oder Stoffströme mit einem Faktor multipliziert wird.

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Hierzu soll das folgende –vereinfachte– Beispiel zum Verständnis dienen: In der Datenbank ist ein Faktor von 1 kg CO₂-eq. pro kWh für den Einsatz von elektrischer Energie aus Braunkohle hinterlegt. Werden jetzt 51 kWh für die Herstellung eines Produktes benötigt und elektrische Energie aus Braunkohle als Energiequelle ausgewählt, so ergibt sich ein GWP von 51 kg CO₂-eq. pro hergestelltes Produkt (z. B. 1 kg H₂) [43].

2.4 Gestehungskosten

Im 3. Artikel werden die Gestehungskosten der Gase berechnet, basierend auf den Stromgestehungskosten (*levelized cost of electricity*). Dabei handelt es sich um eine Methode, um die Kosten von verschiedenen Kraftwerkstypen mit unterschiedlicher Erzeugungs- und Kostenstruktur vergleichbar zu machen. Die Stromgestehungskosten werden in der Einheit €/MWh oder €_{cent}/kWh angegeben und setzen sich im Zähler aus den Investitionskosten, den fixen und variablen Betriebskosten sowie ggf. den Brennstoffkosten und den Kosten für CO₂-Emissionen (*carbon tax*) über den Zeitraum t zusammen. Der Nenner besteht aus der erzeugten Strommenge über den Zeitraum t . Die Werte werden über den Zeitraum t für die einzelnen Jahre diskontiert, da die Stromgestehungskosten nach der Kapitalwertmethode berechnet werden, und anschließend summiert. Danach erfolgt die Division von Zähler und Nenner mit dem Resultat der Stromgestehungskosten. Die Berechnung der Gestehungskosten von Wasserstoff und SNG basiert auf der Berechnung der Stromgestehungskosten und ist entsprechend nach [16,44] angewendet worden.

2.5 Umweltkosten

Neben den Gestehungskosten sind im 3. Artikel die Umweltkosten der Wasserstoff- bzw. SNG-Herstellung berechnet worden. Die Berechnung erfolgt durch die Multiplikation der Umweltauswirkungen (s. Artikel 1 und 2) mit den Umweltpreisen, die von CE Delft veröffentlicht worden sind (s. Tab. 2) [45]. Die Umweltkosten können als Wohlfahrtsverlust und somit als Schadenskosten für die Gesellschaft aufgrund von Umweltbelastungen interpretiert werden. Dies bedeutet, dass aufgrund von ausgestoßenen Emissionen ein Schaden für die Gesellschaft entsteht [46]. Da den Umweltkosten wenig bis gar keine Aufmerksamkeit in klassischen Kostenstudien geschenkt wird, hat der Autor entschieden, die Umweltkosten auf Basis der Umweltpreise von CE Delft zu integrieren, auch deswegen, weil Schäden für die Gesellschaft in Zukunft durch Extremwetterereignisse, die auf erhöhte

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Treibhausgasemissionen in der Atmosphäre zurückzuführen sind, häufiger zu erwarten sind [47]. Daher sieht der Autor die Berechnung der Umweltkosten bei der Herstellung von Wasserstoff und SNG als sinnvolle Ergänzung zur klassischen Kostenberechnung an.

2.6 GWP-Ergebnisse

In dieser Arbeit geben die GWP-Ergebnisse die potenziellen Treibhausgasemissionen der Wasserstoff- und SNG-Herstellung an und werden u. a. mit den CO₂-Emissionen anderer Prozesse verglichen. Die Ergebnisse des GWP werden in der Einheit CO₂-eq. angegeben und umfassen u. a. CO₂-Emissionen, Methan, Lachgas und andere Treibhausgase. Die CO₂-Äquivalente (CO₂-eq.) sind eine Maßeinheit, um die Klimawirkung verschiedener Treibhausgase zu vereinheitlichen.

Im nachfolgenden Abschnitt wird auf den Forschungsstand eingegangen.

3 Forschungsstand

Dieser Abschnitt beschäftigt sich mit dem Forschungsstand zum Dissertationsthema. Dazu wird der Forschungsstand in die Teilbereiche Umweltauswirkungen und Gesteigungs- und Umweltkosten aufgeteilt. Aufgrund der Literaturrecherche lässt sich festhalten, dass den Gesteigungskosten von PtG-Prozessen mehr Aufmerksamkeit geschenkt wird, als den potenziellen Umweltauswirkungen der Prozesse.

3.1 Forschungsstand Umweltauswirkungen

Die wichtigste Studie, auf die sich der Autor für die vergleichende Lebenszyklusanalyse von verschiedenen PtG-Prozessen gestützt hat, ist die Studie von Zhang et al. [37]. Die Studie von Zhang et al. analysiert die potenziellen Umweltauswirkungen von verschiedenen PtG-Prozessen. Dazu sind die Wasserelektrolysetechnologien AEL und PEM sowie verschiedene CO₂-Quellen (Luft, Zementproduktion, elektrische Energieumwandlung aus Biomasse und fossilen Energiequellen), Energieszenarien (Wind, Solar und Energiemix Schweiz/EU) und Wirkungsindikatoren (16 Indikatoren) berücksichtigt worden. Darüber hinaus haben Zhang et al. zwei verschiedene Systemvarianten in ihrer Studie berücksichtigt. Zum einen *subdivision* und zum anderen *system expansion*. *Subdivision* bedeutet, dass ein multifunktionaler Prozess mit mehreren Produkten in separate Prozesse/Produkte unterteilt wird, sodass die mit einem spezifischen Prozess/Produkt einhergehenden Umweltbelastungen eindeutig quantifiziert werden können. Dazu sind die In- und Outputs der Energie- und Stoffströme ausschließlich einem der Produkte zuzuordnen. Diese Methode wird angewendet, um eine Allokation zu vermeiden, wie in der ISO-Norm 14044-2006 empfohlen wird. Hinsichtlich der *system expansion* ist eine Aufteilung in separate Prozesse nicht erforderlich. Stattdessen werden multifunktionale Prozesse mit mehreren Produkten als ein erweitertes System betrachtet [37]. In der vorliegenden Arbeit ist nur die Systemvariante *Subdivision* angewendet worden, um, basierend auf der Empfehlung in der ISO-Norm 14044-2006, Allokationen zu vermeiden.

Zhang et al. fokussieren sich in ihrer Studie auf die potenziellen Treibhausgasemissionen der Wasserstoff- und SNG-Herstellung in verschiedenen PtG-Prozessen, die mit der konventionellen Wasserstoffproduktion sowie der konventionellen Nutzung von Erdgas als Kraftstoff für Fahrzeuge verglichen werden (nur PtM). Zhang et al. schlussfolgern in ihrer Studie, dass nur die Systemvariante *system expansion* mit

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fossilen CO₂-Quellen das volle Potenzial von PtM zur Reduzierung von potenziellen Treibhausgasemissionen als Fahrzeugkraftstoff zeigt. Darüber hinaus schlussfolgern sie, dass das Ersetzen von fossilen durch grünen Wasserstoff mehr zur Reduzierung von Treibhausgasemissionen beitragen kann, als der Ersatz von konventionellem Erdgas durch grünes SNG für den Einsatz als Fahrzeugkraftstoff. Die übrigen Wirkungsindikatoren spielen in der Studie eine untergeordnete Rolle [37].

Gemäß Zhang et al. sind hinsichtlich der potenziellen Umweltauswirkungen von PtG-Technologien bisher nur wenige Studien veröffentlicht worden [25,29,30,37,48-60]. Dabei fokussiert sich die Mehrheit der Studien nur auf PtH, während PtM weniger im Fokus ist, was u. a. einen Vergleich der beiden PtG-Prozesse unter gleichen Bedingungen nach Aussage von Zhang et al. erschwert [37]. Darüber hinaus berücksichtigen die meisten Studien nur biogene CO₂-Quellen, während andere CO₂-Quellen kaum eine Rolle spielen. Außerdem werden in anderen Studien Wirkungsindikatoren –wie radioaktive Strahlung oder Ozonabbau (s. Tab. 1)–, die über das GWP hinausgehen, kaum berücksichtigt [37]. Dass sich die meisten Studien auf den Wirkungsindikator GWP fokussieren und hinsichtlich PtM meistens nur eine biogene CO₂-Quelle einbeziehen, wird auch von Bhandari et al. und Koj et al. bestätigt [56,61], die jeweils eine umfangreiche Literaturrecherche zu den potenziellen Umweltauswirkungen von PtG Prozessen durchgeführt haben. Bhandari et al. stellten in ihrer Literaturrecherche zudem fest, dass die Stromversorgung einen wesentlichen Einfluss auf die potenziellen Umweltauswirkungen der Wasserstoffherstellung hat und, dass der Einsatz von erneuerbaren Energiequellen die Treibhausgasemissionen des gesamten Lebenszyklus erheblich verringert [56]. Aus der Studie von Koj et al. geht des Weiteren hervor, dass die herangezogenen Studien hinsichtlich der potenziellen Umweltauswirkungen von PtG-Prozessen nur eine Wasserelektrolysetechnologie berücksichtigten, wobei der Fokus auf AEL und PEM lag [61]. Zusammen mit einer begrenzten Datenverfügbarkeit, die sich insbesondere auf Daten der PEM- und SOEC-Technologien bezieht [37,55,57], ist dem Autor dieser Arbeit daher keine Studie bekannt, die alle drei wichtigen Wasserelektrolysetechnologien bei der Analyse der potenziellen Umweltauswirkungen von PtG-Technologien in Deutschland berücksichtigt. Daher stellt die vergleichende Lebenszyklusanalyse von potenziellen Umweltauswirkungen bei der Wasserstoff- und SNG-Herstellung in PtG-Prozessen (PtH und PtM), die über das GWP hinausgehen, jeweils einen neuen Beitrag für die wissenschaftliche Gemeinschaft

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dar, unter Berücksichtigung aller drei wichtigen Wasserelektrolysetechnologien, unterschiedlicher CO₂-Quellen sowie verschiedener Energieszenarien für Deutschland.

3.2 Forschungsstand Gestehungs- und Umweltkosten

Wie zu Beginn dieses Kapitels bereits erwähnt, gibt es wesentlich mehr Studien zu den Gestehungskosten von Wasserstoff und SNG als zu den potenziellen Umweltauswirkungen [37]. Dass das Interesse an den Gestehungskosten von Wasserstoff und SNG in den letzten Jahren gestiegen ist, wird vor allem durch die Studien von Dahiru et al. und Yue et al. belegt [28,62]. Gemäß der Studie von Dahiru et al. stieg die Anzahl der Publikationen zum Themenbereich Gestehungskosten von SNG von zwei im Jahr 2010 auf 90 im Jahr 2021 an [62], während nach Yue et al. die Anzahl der Publikationen zum Themenbereich Gestehungskosten von Wasserstoff von 806 im Jahr 2015 auf 1.985 im Jahr 2019 um etwa 146 % zunahm [28]. Die Studien verdeutlichen, dass in diesem Bereich sehr viel Bewegung ist.

Die Berechnung der Gestehungskosten erfolgte mit der Methode von Rubin et al., die in erster Linie für die Berechnung der Gestehungskosten von fossilen Kraftwerksprozessen eingesetzt wird, wobei die Anwendung der Methode auch für die Berechnung der Gestehungskosten von Wasserstoff und SNG geeignet ist [63]. Die Methode von Rubin et al. ist im Vergleich zu anderen Methoden, die in der Literatur für die Berechnung der Gestehungskosten von Wasserstoff und SNG herangezogen worden sind [16-31], detaillierter, da mehr Kostenfaktoren berücksichtigt werden [44]. Der Autor entschied sich die Gestehungskosten von Wasserstoff und SNG nach der Methode von Rubin et al. zu berechnen, um so eine neue Perspektive auf die Gestehungskosten von Wasserstoff und SNG in Deutschland unter Berücksichtigung aller drei wichtigen Wasserelektrolysetechnologien zu ermöglichen, da die Methode erstens vorwiegend nicht für die Berechnung der Gestehungskosten von Wasserstoff und SNG angewendet wird und zweitens, da der Fokus in der Literatur hinsichtlich der Gestehungskosten von Wasserstoff und SNG in erster Linie auf der AEL- und PEM-Technologie (Wasserstoff) bzw. nur einer Wasserelektrolysetechnologie und einer CO₂-Quelle (SNG) liegt [19-21,24,25,28,29,62], was so auch auf Studien übertragen werden kann, die sich nur auf Deutschland beziehen [64-70]. Daher bietet die Berechnung der Gestehungskosten von Wasserstoff und SNG nach der Methode von Rubin et al. nicht nur eine neue Perspektive auf

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ebenjene, sondern auch einen Mehrwert für die wissenschaftliche Gemeinschaft, da, wie im 1. Kapitel bereits erwähnt, dem Autor keine Studie bekannt ist, in der die Methode von Rubin et al. für die Berechnung der Gesteungskosten für Wasserstoff und SNG in Deutschland unter Berücksichtigung der drei wichtigsten Wasserelektrolysetechnologien in einer Studie angewendet worden ist.

Aufgrund der Daten- und Informationslage konnten, wie oben bereits erwähnt, nur gegenwärtige Gesteungskosten und keine Kosten für 2030 oder 2050 berechnet werden. Daher bietet die Studie u. a. eine Grundlage für zukünftige Forschungsarbeiten. Zudem sind in diesem Artikel die Umweltkosten berechnet worden, als sinnvolle Ergänzung einer klassischen Kostenstudie, was einen Mehrwert für die Studie und ihre Leser darstellt. Umweltkosten werden als Schadenskosten für die Gesellschaft aufgrund des voranschreitenden Klimawandels zunehmend eine wichtigere Rolle spielen [45,46]. Die Umweltkosten von Wasserstoff und SNG, die sich, wie im vorherigen Kapitel bereits erwähnt, aus den potenziellen Umweltauswirkungen und Umweltpreisen (s. Tab. 2) zusammensetzen, spielen in der Literatur keine Rolle [71].

Aufgrund dessen, dass der 3. Artikel vor dem Ukrainekrieg und den resultierenden hohen Energiepreisen fertiggestellt wurde und wegen der Daten- und Informationslage keine zukünftigen Werte für 2030 und 2050 berücksichtigt, hat sich der Autor entschieden, zwei weitere Artikel zu den Gesteungskosten von Wasserstoff und SNG mit einer vereinfachten Methode nach Gorre et al. [16] zu verfassen, die auch zukünftige Werte einbeziehen. Da die meisten Studien zu den Gesteungskosten von Wasserstoff und SNG ebenfalls vor dem Ukrainekrieg publiziert worden sind, und somit keine aktuellen Preise für elektrische Energie berücksichtigen konnten, und, wie oben bereits erwähnt, meistens nur eine Wasserelektrolysetechnologie und eine CO₂-Quelle (SNG) oder meistens nur AEL und PEM (Wasserstoff) in die Analyse miteinbezogen, bieten die Artikel jeweils einen neuen Beitrag für die wissenschaftliche Gemeinschaft, da alle drei wichtigen Wasserelektrolysetechnologien, verschiedene CO₂-Quellen, aktuelle Preise für elektrische Energie und Werte für 2030 und 2050 berücksichtigt bzw. berechnet worden sind, um so ein umfassendes Bild der Gesteungskosten für die Wasserstoff- und SNG-Produktion in Deutschland mit einer vereinfachten Methode zu zeigen.

In Kapitel 4 wird auf die Vorgehensweise der Arbeiten eingegangen.

4 Vorgehensweise

In diesem Kapitel werden die Vorgehensweisen zusammenfassend dargestellt, die angewendet worden sind, um die potenziellen Umweltauswirkungen und Geste- hungs- und Umweltkosten der PtG-Prozesse zu ermitteln. Dazu wird das 4. Kapitel in 4.1 Vorgehensweise Umweltauswirkungen und 4.2 Vorgehensweise Geste- hungs- und Umweltkosten unterteilt.

4.1 Vorgehensweise Umweltauswirkungen

Um die potenziellen Umweltauswirkungen der PtG-Technologien und Prozesse zu ermitteln, ist die LCA-Software Umberto+ Version 3.5 zum Einsatz gekommen. Dazu sind Massen- und Energiedaten bezüglich der PtG-Technologien und Pro- zesse erhoben worden, um die Energie- und Stoffströme in der LCA-Software ab- bilden zu können. Die Daten basieren auf Literatur, Herstellerangaben, Experten- meinungen und eigenen Berechnungen sowie auf Hintergrunddaten aus der Ecoin- vent-Datenbank Version 3.5. Die Daten sind, wie in Abschnitt 2.3 beschrieben, in die Software eingefügt worden, um entsprechende LCA-Modelle zu erstellen. Für die Ermittlung der Ergebnisse ist auf die Methode ILCD 2.0 midpoint 2018 zurück- gegriffen worden, abgesehen vom GWP (IPCC 2013). Insgesamt sind folgende Wirkungsindikatoren für die vergleichende Lebenszyklusanalyse der PtG-Techno- logien und Prozesse berücksichtigt worden (s. Tab. 1), um mehr Indikatoren als nur die Wirkungskategorie GWP abzubilden. Eine genaue Beschreibung der einzelnen Indikatoren, ist in den Artikeln zu finden. Die in Tab. 1 aufgelisteten Indikatoren entsprechen entweder dem Level 1 (empfohlen und zufriedenstellend) oder Level 2 (empfohlen, allerdings sind Verbesserungen notwendig), gemäß den Standards des ILCD (International Life Cycle Data system) [72].

Tabelle 1: Übersicht Wirkungsindikatoren

Nr.	Wirkungskategorie	Wirkungsindikatoren	Abkürzung
1	Human health	Ozone Depletion Potential (Ozone layer depletion)	ODP
2	Human health	Carcinogenic effects	CE
3	Human health	Particulate matter (respiratory effects)	PM
4	Human health	Ionizing radiation	IR
5	Human health	Photochemical ozone creation	POC
6	Ecosystem quality	Freshwater & terrestrial acidification	Acid.
7	Ecosystem quality	Freshwater eutrophication	Eutr.
8	Climate change	Global Warming Potential (GWP 100)	GWP

4. Vorgehensweise

Unter Berücksichtigung der drei wichtigsten Wasserelektrolysetechnologien, der verschiedenen CO₂-Quellen und vier verschiedenen Energieszenarien sind insgesamt 120 LCA-Modelle modelliert worden. Abb. 1 zeigt einen Überblick über die PtG-Prozesse.

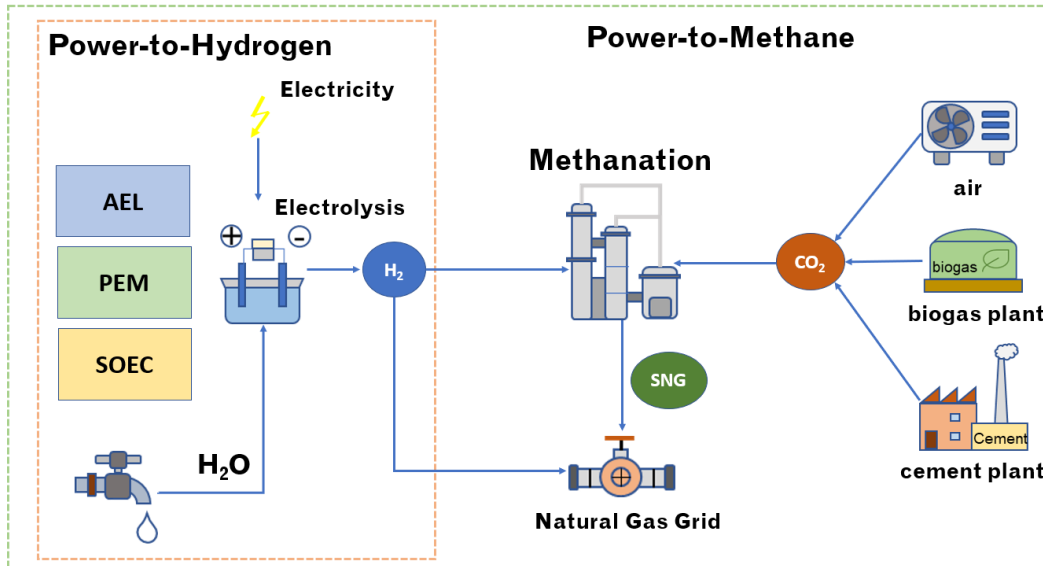


Abbildung 1: Übersicht Power-to-Gas Prozesse

Darüber hinaus zeigt Abb. 2 eine Übersicht über die herangezogenen Energieszenarien für Deutschland, die aus der Literatur entnommen worden sind [55,73,74].

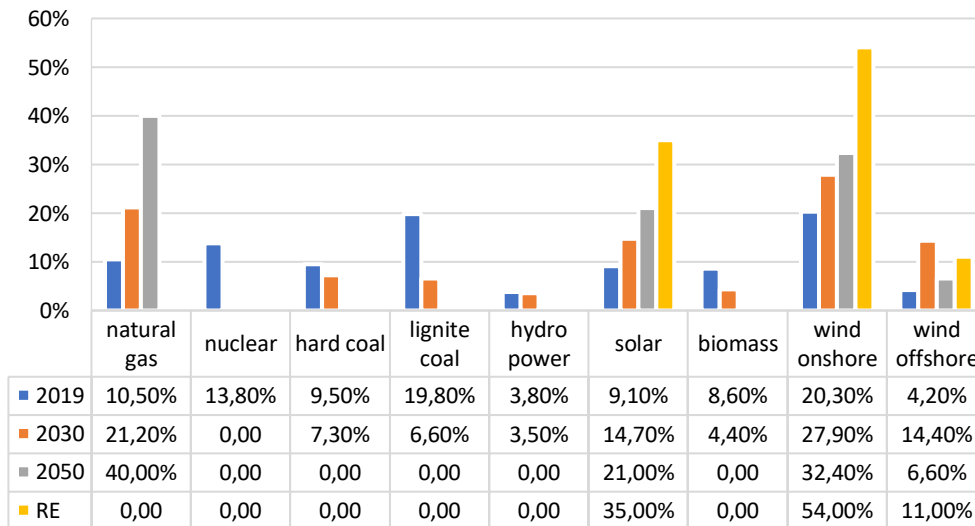


Abbildung 2: Energieszenarien

Wie zu erkennen ist, nehmen die Anteile von Wind- und Solarenergie am Energiemix von 2019 bis 2050 stetig zu. Des Weiteren gibt es nach 2030 keinen Anteil von Braun- und Steinkohle am Energiemix mehr. Auffällig ist auch, dass der Anteil an Erdgas bis 2050 zunimmt. Dies hängt damit zusammen, dass Erdgas als

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Übergangslösung gesehen wird, um die schwankende Verfügbarkeit von Wind- und Solarenergie auszugleichen [55], da Gaskraftwerke kurzfristig eingesetzt werden können. An dieser Stelle noch eine Anmerkung, dass sich die Anteile von Braun- und Steinkohle am Energiemix 2030 noch ändern können, was insbesondere vom Zeitpunkt des Kohleausstiegs abhängig ist.

4.2 Vorgehensweise Gesteigungs- und Umweltkosten

Die Methode von Rubin et al. ist eine detaillierte und wissenschaftlich anerkannte Methode zur Berechnung der Gesteigungskosten von fossilen Kraftwerksprozessen, die auch für PtG-Prozesse angewendet werden kann [44,63]. Die Daten für die Berechnung der Gesteigungskosten von Wasserstoff und SNG basieren entweder auf Herstellerangaben, eigenen Schätzungen oder Literaturwerten und sind in die Methode von Rubin et al. integriert worden. Dabei stellen die Bare Erected Cost (BEC) nach Aussage von Rubin et al. den wichtigsten Teil der Kostenanalyse dar [44]. Die BEC umfassen Kosten für die Prozessausrüstung, unterstützenden Einrichtungen sowie direkten und indirekten Arbeitskosten. Addiert man diese Kosten zusammen mit den Kosten für Planung, Beschaffung/Bau und Projekt-/Prozesskontingenzen sowie Eigentümerlasten, so ergeben sich die Total Overnight Cost (TOC). Die TOC ergeben zusammen mit der Mehrwertsteuer und eines berücksichtigten Anstiegs für Zinsen und Kosten während des Baus die gesamten Kapitalkosten (Total As-Spent Capital) [44]. Die Kapitalkosten werden zusammen mit den fixen und variablen Instandhaltungs- und Betriebskosten auf das Ausgangsjahr abgezinst und durch die ebenfalls auf das Ausgangsjahr abgezinste Energiemenge (z. B. kWh, MWh oder kg SNG/H₂) geteilt, sodass sich die Gesteigungskosten ergeben [44]. Die Gesteigungskosten geben den Verkaufspreis an, der mindestens erreicht werden muss, um Verluste zu vermeiden, sodass es sich hierbei um den *Break-Even* Preis handelt [75]. Die berücksichtigte Energiemenge basiert auf Daten und Berechnungen von [37,76]. Eine umfassendere Beschreibung der Vorgehensweise kann in Artikel 3 gefunden werden. Die Berechnung der Gesteigungskosten erfolgte für 1 und 100 MW-Anlagen, da die Datenlage für 1 MW-Anlagen sehr gut war und die Erzeugung zukünftig in großen zentralen Anlagen erwartet wird [77]. Die Werte für die 1 MW-Anlagen sind auf die Werte für 100 MW-Anlagen hochskaliert worden, wozu unterschiedliche Skalierungsfaktoren herangezogen worden sind (s. Artikel 3).

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Die Methode von Gorre et al., die in den Artikeln 4 und 5 zur Anwendung kommt, unterscheidet sich insofern von der Methode nach Rubin et al., dass weniger Kostenfaktoren berücksichtigt werden und diese daher weniger detailliert ist. So werden z. B. keine Kosten für unterstützende Einrichtungen, Projekt-/Prozesskontingenzen, Eigentümerlasten sowie direkte und indirekte Arbeitskosten berücksichtigt. Daher handelt es sich bei der Methode von Gorre et al. um eine vereinfachte Methode für die Berechnung von Gestehungskosten [16].

Hinsichtlich der Berechnung der Umweltkosten sind folgende Umweltpreise, die von CE Delft veröffentlicht worden sind [46], herangezogen worden (Tab. 2). Diese Umweltpreise sind mit den Ergebnissen der potenziellen Umweltauswirkungen der Wasserstoff- und SNG-Herstellung aus den Artikeln 1 und 2 multipliziert worden, sodass entsprechende Umweltkosten resultieren.

Tabelle 2: Umweltpreise CE Delft

Impact category	unit ReCiPe	unit ILCD/IPCC	2015	2019
Climate change	€/kg CO ₂ -eq.	€/kg CO ₂ -eq.	0.0566	0.0649
Ozone layer depletion	€/kg CFC-eq.	€/kg CFC-eq.	30.4	30.4
Human toxicity	€/kg 1.4 db-eq.	CTUh	0.0991	0.0991
Particulate matter formation	€/kg PM _{2.5} -eq.	€/kg PM _{2.5} -eq.	39.2	39.2
Ionizing radiation	€/kg kBq U ²³⁵ -eq.	€/kg kBq U ²³⁵ -eq.	0.0461	0.0461
Photochemical oxidant formation	€/kg NMVOC-eq.	€/kg NMVOC-eq.	1.15	1.15
Acidification	€/kg SO ₂ -eq.	mol H ⁺ -eq.	4.97	4.97
Freshwater eutrophication	€/kg P-eq.	€/kg P-eq.	1.86	1.86

Im nachfolgenden Abschnitt geht es um die Zusammenführung der Einzelergebnisse und neue Erkenntnisse der eigenen Arbeit.

5 Publikationen des Autors

Dieser Abschnitt beschäftigt sich mit der Zusammenführung der Ergebnisse und neuen Erkenntnissen der Arbeit. Dazu wird dieser Abschnitt in zwei Teilbereiche gegliedert. Zum einen der Abschnitt potenzielle Umweltauswirkungen von PtG-Prozessen und zum anderen der Abschnitt Gestehungs- und Umweltkosten von PtG-Prozessen.

5.1 Potenzielle Umweltauswirkungen von PtG-Prozessen

Wie im 1. Kapitel bereits erwähnt, beschäftigen sich die ersten beiden Artikel mit den potenziellen Umweltauswirkungen der Wasserstoff- und SNG-Herstellung in PtG-Prozessen. Dabei liegt der Fokus auf dem Wirkungsindikator GWP, dem wichtigsten Indikator bezüglich der potenziellen Umweltauswirkungen von PtG-Prozessen in der Literatur [37]. Aus diesem Grund sind u. a. die verschiedenen PtG-Prozesse mit den unterschiedlichen Technologien (AEL, PEM, und SOEC) und CO₂-Quellen (Luft, Biomasse und Zementherstellung) hinsichtlich des GWP verglichen worden. Darüber hinaus sind die Ergebnisse des GWP im Vergleich zu den Ergebnissen aus anderen Studien und Prozessen eingeordnet und mit den CO₂-Emissionen von konventionellen Energiequellen und Kraftstoffen verglichen worden, unter der Annahme, dass die hergestellten Gase wieder zur Umwandlung in elektrische Energie und als Kraftstoff für Autos eingesetzt werden. Außerdem sind die verschiedenen PtG-Prozesse und Technologien in einer vergleichenden Lebenszyklusanalyse unter Berücksichtigung der unterschiedlichen Energieszenarien und Wirkungsindikatoren (s. Tab. 1) miteinander verglichen worden, um den umweltfreundlichsten Prozess bzw. die umweltfreundlichste Technologie zu identifizieren. Insgesamt lassen sich die Forschungsfragen der Artikel wie folgt zusammenfassen:

1. Welche PtG-Technologie verursacht die geringsten potenziellen Treibhausgasemissionen für das jeweilige Energieszenario und wie lassen sich die Ergebnisse im Vergleich zu anderen Studien bzw. anderen Prozessen einordnen?
2. Wie lassen sich die potenziellen Treibhausgasemissionen der Gase im Vergleich zu den CO₂-Emissionen konventioneller Energiequellen und Kraftstoffe für das jeweilige Energieszenario einordnen, unter der Annahme, dass

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die erzeugten Gase wieder zur Umwandlung in elektrische Energie oder als Kraftstoff für Autos eingesetzt werden?

3. Welche PtG-Technologie ist unter Berücksichtigung aller untersuchten Indikatoren die potenziell umweltfreundlichste für das jeweilige Szenario?

In Bezug auf die SNG-Herstellung ist ein Umweltkredit in Höhe von 1 kg CO₂ pro kg gebundenes CO₂ in SNG berücksichtigt worden, welches in das Erdgasnetz eingespeist wird. Der Grund ist, dass das gebundene CO₂ entweder der Atmosphäre entzogen (CO₂-Quelle Luft, Biomasse) oder nicht in die Atmosphäre ausgestoßen wird (CO₂-Quelle Zementherstellung), und das erzeugte SNG gespeichert und daher nicht direkt genutzt wird. So ergibt sich ein Umweltkredit für das gespeicherte SNG.

Als funktionelle Einheit ist 1 kg H₂ bzw. SNG berücksichtigt worden. Dies bedeutet, dass sich die potenziellen Umweltauswirkungen auf 1 kg des hergestellten Produktes beziehen. Die Angabe einer funktionellen Einheit ist für die Berechnung erforderlich. Darüber hinaus ist aus der Analyse des GWP für die SNG-Herstellung in 1, 5, und 10 MW-Anlagen hervorgegangen, dass sich die Resultate nur sehr geringfügig unterscheiden, was auch von Parra et al. [25] bestätigt wird. Aus diesem Grund hat sich die Analyse der weiteren Indikatoren und die Analyse der PtH-Prozesse nur auf 1 MW-Anlagen beschränkt, da kein Mehrwert in der Analyse von 5 oder 10 MW-Anlagen zu erkennen war. Gemäß Parra et al. trifft dies auch auf größere Anlagen zu [25].

5.1.1 Forschungsfrage 1: Potenzielle Treibhausgasemissionen

Bezüglich der 1. Forschungsfrage kann festgehalten werden, dass PtG-Prozesse mit der SOEC-Technologie die geringsten potenziellen Treibhausgasemissionen für die Energieszenarien 2019, 2030 und 2050 aufweisen, da der spezifische Energiebedarf für PtG-Prozesse mit dieser Technologie geringer ist als mit der AEL- oder PEM-Technologie [76] und somit weniger CO₂-eq. verursacht werden. Dies ändert sich jedoch bei Anwendung des EE-Szenarios, da erstens keine fossilen Brennstoffe mehr im Energiemix enthalten sind, sodass ein höherer Energiebedarf weniger Auswirkungen auf die potenziellen Treibhausgasemissionen hat. Und zweitens, da die Berücksichtigung einer externen Wärmequelle mit Erdgas für PtG-Prozesse mit der SOEC-Technologie bei den Ergebnissen nun stärker ins Gewicht fällt. Die Berücksichtigung der externen Wärmequelle für SOEC erfolgte gemäß Mehmeti et al.

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[59], die Erdgas auch als Wärmequelle für SOEC in EE-Szenarien (Wind- und Sonnenenergie) angenommen haben. Die Annahme einer fossilen Wärmequelle in einem zukünftigen EE-Szenario ist allerdings kritisch zu hinterfragen, insbesondere vor dem Hintergrund der Klimaziele, und sollte in zukünftigen Forschungsarbeiten entsprechend berücksichtigt werden. Für das EE-Szenario verursachen PtG-Prozesse mit der AEL-Technologie am wenigsten CO₂-eq., wobei sich die potenziellen Treibhausgasemissionen im Vergleich zu PtG-Prozessen mit der PEM-Technologie kaum unterscheiden.

Darüber hinaus kann festgehalten werden, dass die potenziellen Treibhausgasemissionen in guter Übereinstimmung mit einzelnen Literaturwerten aus Peer-Studien sind [37,52,53,55,59,78]. Es ist allerdings darauf hinzuweisen, dass ein Vergleich mit Peer-Studien nur sehr eingeschränkt möglich ist, da unterschiedliche Annahmen und Szenarien getroffen bzw. berücksichtigt worden sind, was z. T. erhebliche Auswirkungen auf die Ergebnisse hat.

Werden die potenziellen Treibhausgasemissionen für Wasserstoff mit konventionellen Herstellungsprozessen verglichen, so lässt sich festhalten, dass die potenziellen Treibhausgasemissionen der 2030er- und 2050er-Szenarien zwischen den in der Literatur ausgewiesenen Werten für *steam methane reforming* und *coal gasification* liegen und nur die potenziellen Treibhausgasemissionen des EE-Szenarios niedriger sind als die berücksichtigten Vergleichsprozesse (s. Artikel 1), sodass sich mit dem Ersatz von fossilen durch grünen Wasserstoff erhebliche Reduktionspotenziale von Treibhausgasemissionen ergeben würden, was so auch von Zhang et al [37] bestätigt wird. In Bezug auf Biomasse-basierten Vergleichsprozessen lässt sich festhalten, dass der Wert für *dark fermentation* auf dem Niveau der 2050er-Werte liegt, während der Wert für *biomass-derived liquid reforming* zwischen den Werten des 2050er-Szenarios und den Werten des EE-Szenarios liegt (s. Artikel 1). Außerdem sind die potenziellen Treibhausgasemissionen der SNG-Herstellung mit den CO₂-Emissionen der konventionellen Erdgasproduktion verglichen worden. Diesbezüglich sind die CO₂-Emissionen der konventionellen Erdgasproduktion erheblich niedriger als die potenziellen Treibhausgasemissionen der SNG-Herstellung und nur die potenziellen Treibhausgasemissionen im EE-Szenario sind niedriger als die CO₂-Emissionen der konventionellen Erdgasproduktion, nachdem der Umweltkredit (siehe oben) berücksichtigt worden ist (s. Artikel 2).

Des Weiteren ist in den Studien detaillierter auf die Wirkungsindikatoren und deren Veränderung hinsichtlich der Energieszenarien eingegangen worden, worauf in dieser Zusammenfassung nicht eingegangen wird.

5.1.2 Forschungsfrage 2: Elektrische Energie und Kraftstoff

Hinsichtlich der 2. Forschungsfrage ist untersucht worden, wie sich die potenziellen Treibhausgasemissionen von Wasserstoff und SNG im Vergleich zu den CO₂-Emissionen von elektrischer Energie, die aus konventionellen Energiequellen umgewandelt wurde, und konventionellen Kraftstoffen einordnen lassen, unter der Annahme, dass die aus elektrischer Energie erzeugten Gase wieder zur Umwandlung in elektrische Energie bzw. als Kraftstoff für Autos genutzt werden. Dazu sind die Ergebnisse bezüglich der Umwandlung in elektrische Energie durch 33.33 kWh/kg-H₂ (*Lower-Heating-Value*, H₂) und 15.4 kWh/kg-SNG (*Higher-Heating-Value*, CH₄) geteilt worden [79,80], um Ergebnisse pro kWh zu erhalten, während bezüglich des Einsatzes als Kraftstoff für Autos angenommen worden ist, dass die Reichweite von 1 kg H₂ 100 km und von 1 kg SNG 19.5 km beträgt [37,81]. Diese Werte sind entsprechend herangezogen worden, um Werte pro km zu erhalten.

Für den Vergleich des Einsatzes von Wasserstoff und SNG zur Umwandlung in elektrische Energie sind Braun- und Steinkohle, Erdgas, Erdgas aus der Ecoinvent-Datenbank und der Energiemix von 2019 als konventionelle Energiequellen herangezogen worden. Dabei ist der Wert aus der Ecoinvent-Datenbank herangezogen worden, da dieser Wert in der Einheit kg CO₂-eq. angegeben wird und somit die gleiche Einheit wie die GWP-Ergebnisse hat.

Wie in den Abb. 3 und 4 zu erkennen ist, liegen nur die potenziellen Treibhausgasemissionen der mit EE hergestellten Gase unter den CO₂-Emissionen der konventionellen Energiequellen, sodass sich hier ein Reduktionspotenzial von Treibhausgasemissionen ergibt, wenn die zur langfristigen Speicherung von elektrischer Energie hergestellten Gase z. B. im Winter –anstatt der Nutzung von konventioneller Energiequellen– wieder in elektrische Energie umgewandelt werden. Die potenziellen Treibhausgasemissionen des 2050er-Szenarios liegen im Bereich der Werte für Erdgas (u. a. wegen des hohen Erdgasanteils, s. Abb. 2), während die Werte für die 2019er- und 2030er-Szenarien kleiner als die Werte für Braun- und Steinkohle sind, allerdings über oder in dem Bereich der übrigen Vergleichswerte liegen.

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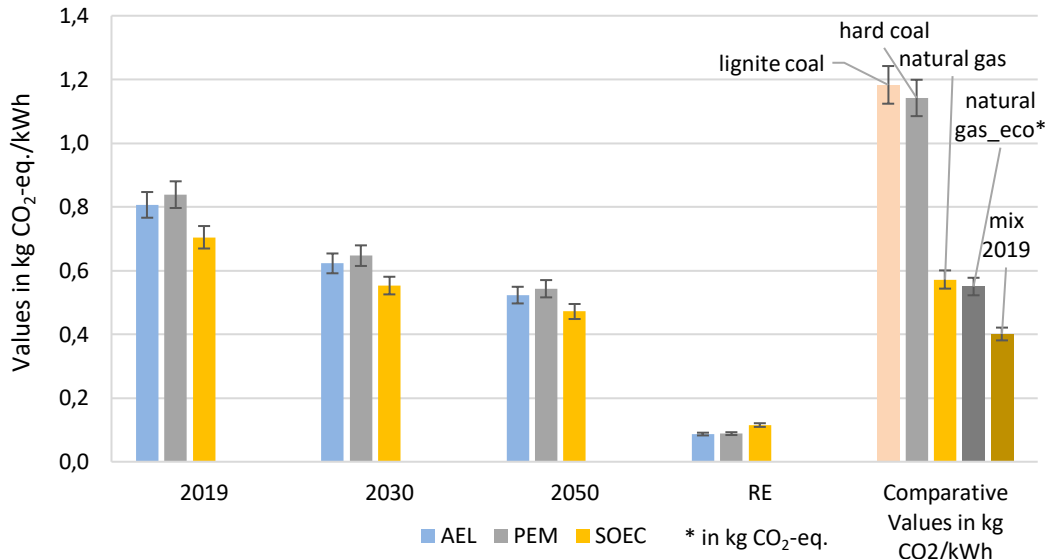


Abbildung 3: H₂ im Vergleich zu konventionellen Werten (elektr. Energie)

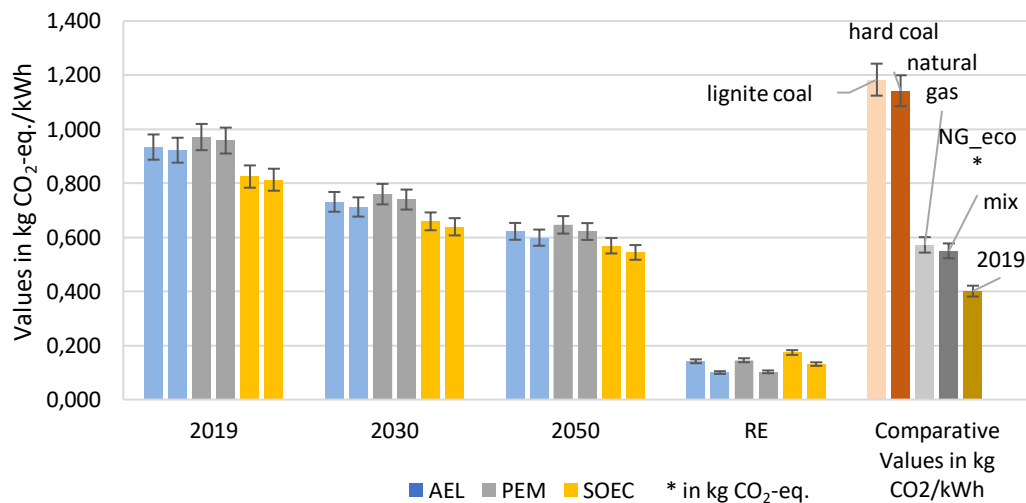


Abbildung 4: SNG im Vergleich zu konventionellen Werten (elektr. Energie)

Die Abb. 5 und 6 zeigen den Vergleich der potenziellen Treibhausgasemissionen, der in den verschiedenen PtG-Prozessen hergestellten Gase, mit den CO₂-Emissionen der berücksichtigten konventionellen Kraftstoffe, unter der Annahme, dass Wasserstoff und SNG als Kraftstoff für Autos eingesetzt werden. Dazu sind Benzin, Diesel, Flüssiggas und komprimiertes Erdgas als konventionelle Energiequellen berücksichtigt worden.

Wie aus den Abbildungen zu erkennen ist, sind nur die potenziellen Treibhausgasemissionen des EE-Szenarios geringer als die CO₂-Emissionen der konventionellen Vergleichswerte (abgesehen von CNG), während die übrigen potenziellen

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Treibhausgasemissionen der anderen Szenarien ungefähr gleichauf oder deutlich über diesen Werten liegen.

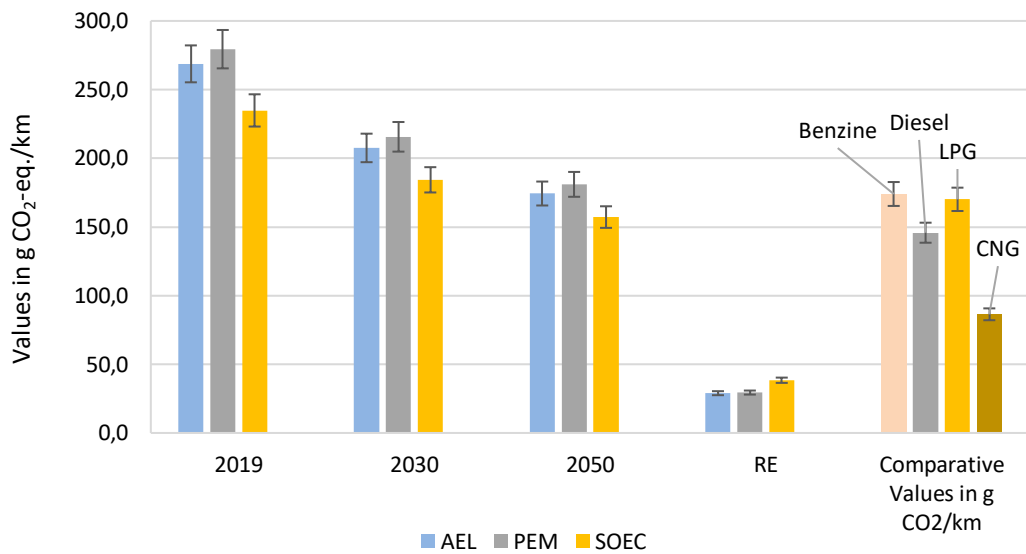


Abbildung 5: H₂ im Vergleich zu konventionellen Werten (Kraftstoff)

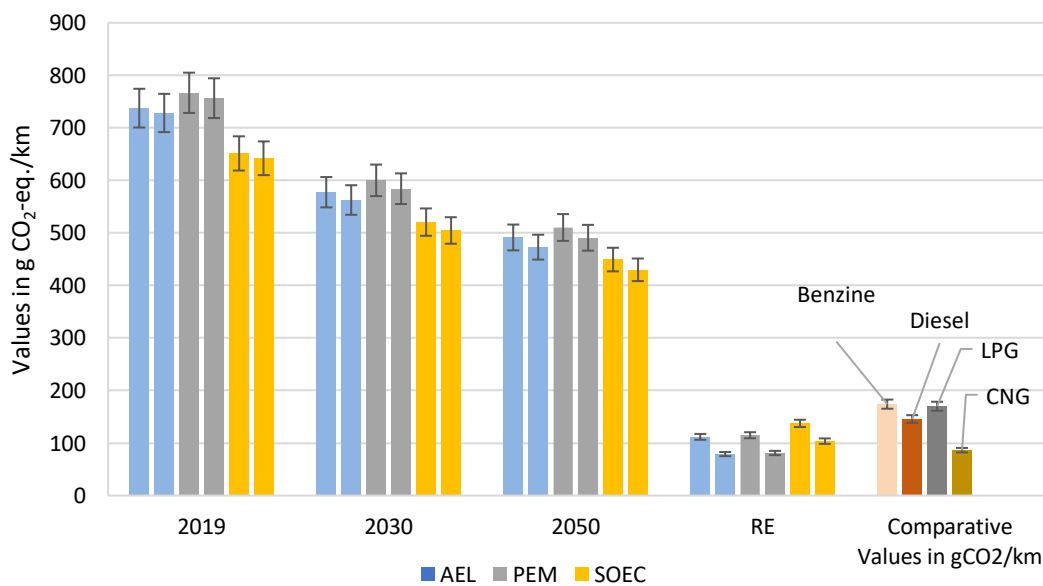


Abbildung 6: SNG im Vergleich zu konventionellen Werten (Kraftstoff)

Insgesamt bleibt daher festzuhalten, dass in dieser Analyse nur die aus 100 % EE hergestellten Gase ein Reduktionspotenzial von Treibhausgasemissionen aufweisen, wenn diese z. B. im Winter –anstatt konventioneller Alternativen– wieder in elektrische Energie umgewandelt oder als Kraftstoff für Autos eingesetzt werden. Was aus den Ergebnissen noch hervorgeht, ist, dass insbesondere grüner

Wasserstoff einen erheblichen Teil dazu beitragen kann, um Treibhausgasemissionen zu reduzieren, wenn dieser primär als Ersatz für konventionelle Energiequellen (z. B. Erdgas) eingesetzt wird. Daher kann grüner Wasserstoff als Schlüsselement einen signifikanten Beitrag zur Milderung des Klimawandels beitragen. Aus diesem Grund wird grünem Wasserstoff eine besondere Rolle für die zukünftige Energieversorgung Deutschlands beigemessen (s. Kapitel 2).

5.1.3 Forschungsfrage 3: Umweltfreundlichster Prozess

Der Fokus der 3. Forschungsfrage lag darauf, zu ermitteln, welche PtG-Technologie unter Berücksichtigung aller Wirkungsindikatoren (s. Tab. 1) die umweltfreundlichste Technologie für das jeweilige Szenario ist. Dazu sind alle Wirkungsindikatoren gleich gewichtet und die Ergebnisse für die Technologien untereinander ins Verhältnis gesetzt worden. Die Abbildungen, die die Ergebnisse veranschaulichen, können in den einzelnen Studien nachgeschlagen werden (s. Artikel 1 und 2).

Hinsichtlich der PtH-Prozesse kann die SOEC-Technologie als die umweltfreundlichste Elektrolysetechnologie für das 2019er- und das 2030er-Szenario klassifiziert werden, während dies auf die PEM-Technologie für das 2050er- und das EE-Szenario zutrifft. Die Gründe dafür, dass die SOEC-Technologie nicht mehr die umweltfreundlichste Technologie ist, sind schon in Abschnitt 5.1.1 thematisiert worden und zwar, dass der Anteil an Wind- und Solarenergie stetig zunimmt und die externe Wärmequelle mit Erdgas (CO₂-Emissionen) dadurch stärker ins Gewicht fällt. Die AEL-Technologie, die für das GWP im EE-Szenario den geringsten Wert verursacht (s. Abschnitt 5.1.1), ist für alle Szenarien die umweltunfreundlichste Technologie, u. a. aufgrund des hohen Stahl- und Nickelbedarfs, die hohe potenzielle Umweltauswirkungen im Bereich krebserregende Wirkung und Versauerung von Frischwasser und Böden nach sich ziehen.

Das gleiche trifft auch auf die Herstellung von SNG zu. So ist die Herstellung unter Berücksichtigung der Szenarien 2019 und 2030 mit der SOEC-Technologie für alle CO₂-Quellen am umweltfreundlichsten, während dies auf die PEM-Technologie für die Szenarien 2050 und das EE-Szenario zutrifft, abgesehen vom 2050er-Szenario mit Biomasse als CO₂-Quelle, wo keine klare Aussage getroffen werden kann. Insgesamt lässt sich daher festhalten, dass die Produktion von Wasserstoff und SNG aus Umweltgesichtspunkten mit der SOEC-Technologie für die Szenarien 2019 und

2030 durchgeführt werden sollte, während dies auf die PEM-Technologie für 2050 und das EE-Szenario zutrifft.

5.2 Neue Erkenntnisse zum Umweltbereich

Die Berücksichtigung aller drei wichtigen Wasserelektrolysetechnologien, verschiedener CO₂-Quellen sowie unterschiedlicher Energieszenarien und mehr Wirkungsindikatoren als nur das GWP liefern neue Erkenntnisse hinsichtlich der potenziellen Umweltauswirkungen von PtG-Prozessen. So konnte in den umfassenden Studien ermittelt werden, welcher PtG-Prozess bzw. welche PtG-Technologie für das jeweilige Szenario der umweltfreundlichste Prozess bzw. die umweltfreundlichste Technologie ist. Die neuen Erkenntnisse in Bezug auf die potenziellen Umweltauswirkungen von PtG-Prozessen können als Entscheidungsgrundlage für die Implementierung zukünftiger PtG-Prozesse dienen, vor allem da Umweltauswirkungen und die daraus resultierenden gesellschaftlichen Schadenskosten immer mehr in den Vordergrund rücken. Darüber hinaus bieten die erstellten LCA-Modelle eine solide Datengrundlage, insbesondere vor dem Hintergrund, dass die Datengrundlage für PEM und SOEC begrenzt war. Zudem können die erstellten LCA-Modelle leicht adaptiert werden, z. B. hinsichtlich der Energieszenarien in anderen Ländern. Daher bieten die erstellten LCA-Modelle neben einer soliden Datengrundlage auch die Möglichkeit für weitere Forschungsarbeiten.

Neue Erkenntnisse sind auch hinsichtlich des Vergleichs der potenziellen Treibhausgasemissionen der Gase mit den CO₂-Emissionen konventioneller Energiequellen und Kraftstoffe entstanden, wenn die Gase wieder zur Umwandlung in elektrische Energie oder als Kraftstoff für Autos eingesetzt werden. So verursachen nur die im EE-Szenario erzeugten Gase z. T. erheblich weniger Netto-Emissionen über alle Technologien hinweg im Vergleich zu konventionellen Alternativen, wenn sie wieder zur Umwandlung in elektrische Energie oder als Kraftstoff für Autos eingesetzt werden (abgesehen von SNG als Kraftstoff im Vergleich mit komprimiertem Erdgas). Zudem können die Ergebnisse u. a. dazu genutzt werden, um die Einsparungen an Emissionen für eine entsprechende Strecke zu ermitteln, wenn anstatt eines konventionellen Kraftstoffs z. B. grüner Wasserstoff als Kraftstoff verwendet wird.

5.3 Gesteigungs- und Umweltkosten von PtG-Prozessen

Im 3. Artikel sind die Gesteigungs- und Umweltkosten der PtG-Prozesse berechnet worden. Dazu ist für die Berechnung der Gesteigungskosten die Methode von Rubin et al. angewendet worden, während die Berechnung der Umweltkosten auf Grundlage der veröffentlichten Umweltpreise von CE Delft basiert (s. Tab. 2). Die Berechnung der Gesteigungskosten von Wasserstoff und SNG erfolgte für 1 und 100 MW-Anlagen. Wie eingangs erwähnt, konnten aufgrund der Daten- und Informationslage keine Werte für die Zukunft ermittelt werden. Für die Berechnung der Gesteigungskosten wurden vier verschiedene Szenarien (8000 h Netzenergie, 2000 h Netzenergie, 2000 h Wind- bzw. Solarenergie) für den Bezug von elektrischer Energie berücksichtigt. Dabei ist angenommen worden, dass der Bezug von elektrischer Energie direkt aus erneuerbaren Quellen stammt, wozu jeweils 2000 h für Wind- (onshore) und Solarenergie nach [82,83] angenommen worden sind.

Die Studie kommt zu dem Ergebnis, dass die Gesteigungskosten von Wasserstoff in 100 MW-Anlagen um 27 % (8,000 h, Netzenergie), 45 % (2000 h, Netzenergie) und 50-58 % (2,000 h, Wind/Solar) geringer sind als in 1 MW-Anlagen und im Bereich zwischen 14-17 €/kg-H₂ (8,000 h, Netzenergie), 25,2-27,3 €/kg-H₂ (2,000 h, Netzenergie) und 16,9-19 €/kg-H₂ (2,000 h, Wind/Solar) liegen.

In Bezug auf SNG sind die Gesteigungskosten in 100 MW-Anlagen um bis zu 51 % (8,000 h, Netzenergie), 65 % (2000 h, Netzenergie) und 70-71 % (2,000 h, Wind/Solar) geringer als in 1 MW-Anlagen und liegen im Bereich zwischen 4,1-12,2 €/kg-SNG (8,000 h, Netzenergie), 7,9-25,6 €/kg-SNG (2000 h, Netzenergie) und 6,1-20,8 €/kg-SNG (2,000 h, Wind/Solar). Dabei sind die Gesteigungskosten für SNG mit Biomasse als CO₂-Quelle im Vergleich zu den anderen CO₂-Quellen am geringsten, was daran liegt, dass das im Biogas enthaltene Methan (angenommener Anteil von 53 % [84]) ebenfalls als SNG eingestuft wird, was zu höheren Produktionsmengen führt, die die Gesteigungskosten trotz der berücksichtigten Kosten für die Biogasproduktion deutlich reduzieren. Außerdem sind die Gesteigungskosten von PtM-Anlagen mit Luft als CO₂-Quelle am höchsten, da die CAPEX für die CO₂-Abtrennungsanlage hoch sind und nach eigenen Schätzungen, die auf Informationen des Start-up-Unternehmens Climeworks [85] beruhen, etwa 5.000 €/kW für 1 MW-PtM-Anlagen betragen. Diese Kosten reduzieren sich aufgrund von Skalierungseffekten auf ca. 1.500 €/kW für 100 MW-Anlagen.

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Die Gesteungskosten von Wasserstoff und SNG sind im Vergleich zu Peer-Studien, die eine vereinfachte Methode angewendet haben, als sehr hoch zu bewerten [16-30]. Der Grund dafür ist, dass die Methode von Rubin et al. mehr Kostenfaktoren, wie z. B. Projekt- und Prozesskontingenzen (s. o.), berücksichtigt.

In Bezug auf die Berechnung der Umweltkosten sind die Umweltauswirkungen des 2019er-Szenarios aus den ersten beiden Artikeln genommen und mit den veröffentlichten Umweltpreisen von CE Delft (s. Tab. 2) multipliziert worden, um gegenwärtige Werte zu ermitteln. Darüber hinaus sind die LCA-Modelle so modifiziert worden, um die Umweltauswirkungen für den direkten Bezug von Wind- und Solarenergie zu ermitteln, sodass auch hierfür die Umweltkosten berechnet werden konnten. Die Ergebnisse beziehen sich jeweils auf 1 kg des hergestellten Produktes und sind in den Abb. 7 und 8 zu sehen.

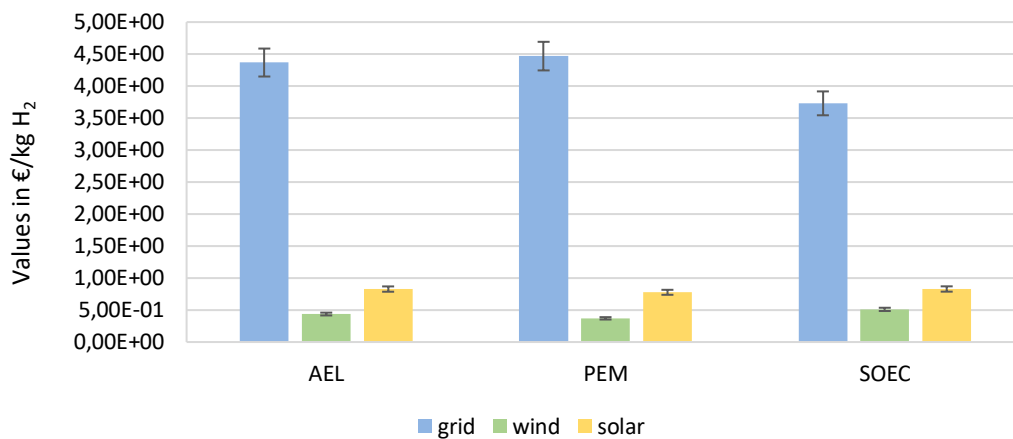


Abbildung 7: Umweltkosten der Wasserstoffherzeugung

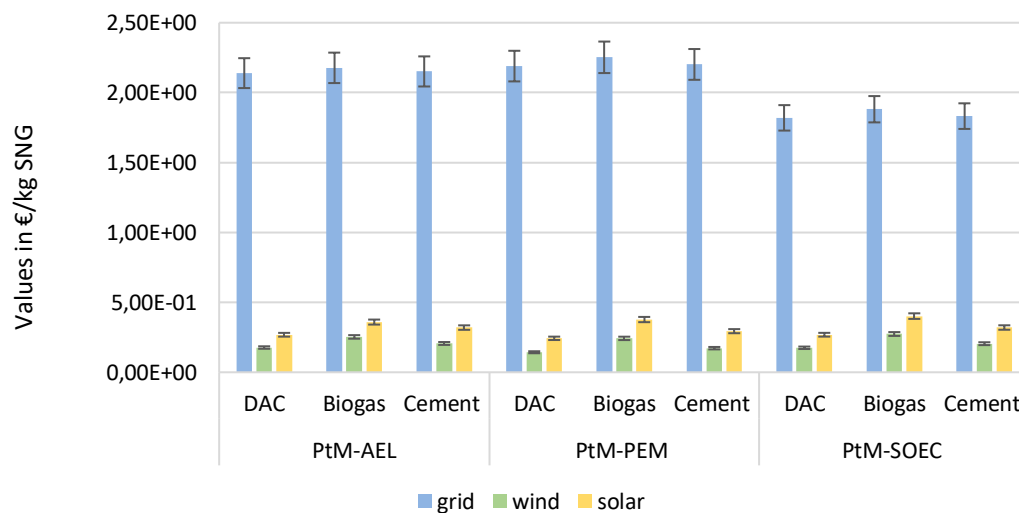


Abbildung 8: Umweltkosten der SNG-Erzeugung

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Wie zu erkennen ist, führt der Bezug von elektrischer Energie aus dem Netz zu wesentlich höheren Umweltkosten, als die Herstellung mit Wind- oder Solarenergie, wobei die Herstellung aus Wind- gegenüber Solarenergie zu bevorzugen ist. Darüber hinaus ist zu erkennen, dass sich die Umweltkosten unter Berücksichtigung aller Wirkungsindikatoren zwischen den einzelnen Technologien nur geringfügig unterscheiden, wenn Wind- oder Solarenergie bezogen wird.

Berechnet man die Umweltkosten für Wasserstoff nur mit dem Wirkungsindikator GWP und vergleicht die Ergebnisse mit den Umweltkosten der Dampfreformierung (nur CO₂-Emissionen konnten berücksichtigt werden), so entsteht folgendes Bild (s. Abb. 9). Die Umweltkosten für die Dampfreformierung sind wesentlich höher als die Umweltkosten für Wasserstoff, der mit Wind- oder Solarenergie hergestellt wird. In diesem Zusammenhang könnte auf Basis der Umweltkosten z. B. eine Umweltsteuer implementiert werden, die darauf abzielt, nachhaltige Prozesse zu fördern. Dazu könnte z. B. die Differenz der Umweltkosten zwischen grünen und fossil hergestellten Wasserstoff herangezogen werden. Da es sich bei der Dampfreformierung um die Herstellung von Wasserstoff aus Erdgas handelt, mit dem mehr als 90 % des weltweiten Wasserstoffs hergestellt werden [86], könnten mit der Implementierung einer etwaigen Umweltsteuer erhebliche Mengen an CO₂-Emissionen eingespart werden, wenn dieser Prozess dadurch wirtschaftlich unattraktiver wird, was in Zeiten des Klimawandels vorteilhaft wäre. Hierzu könnten sogar mehr Wirkungsfaktoren als die CO₂-Emissionen berücksichtigt werden, mit der Konsequenz, dass eine mögliche Umweltsteuer noch höher ausfallen könnte.

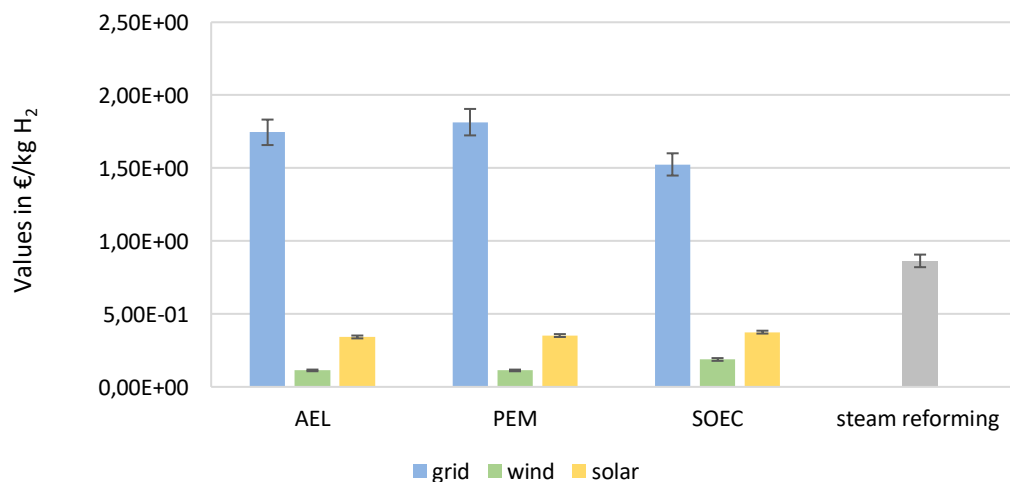


Abbildung 9: Umweltkosten von H₂ im Vergleich zur Dampfreformierung

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Außerdem könnten die Subventionen für fossile Energien, die in Deutschland 16 Mrd. Euro betragen [87] und in Zeiten des Klimawandels nur schwer zu rechtfertigen sind, in die Senkung der Kosten für elektrische Energie investiert werden, die eine Hauptkomponente der Gestehungskosten sind. Wird der Preis für elektrische Energie für das 8.000 h-Szenario z. B. um 50 % von ca. 17 ct/kWh auf 8,5 ct/kWh gesenkt, sinken die Gestehungskosten um ca. 16 % (für 1 MW-PtM-Anlagen), 28 % (für 100 MW-PtM-Anlagen), 25 % (1 MW-PtH-Anlagen) und 34 % (für 100 MW-PtH-Anlagen), was eine erhebliche Verringerung der Gestehungskosten bedeuten würde.

5.4 Neue Erkenntnisse zum Kostenbereich

Die Ergebnisse, die mit der Methode von Rubin et al. ermittelt worden sind, ermöglichen eine neuer Perspektive auf die Gestehungskosten von Wasserstoff und SNG in Deutschland, da diese Methode im Vergleich zu anderen Methoden detaillierter ist und vorwiegend nicht für die Berechnung der Gestehungskosten von Wasserstoff und SNG angewendet wird. Die Methode berücksichtigt im Vergleich zu vereinfachten Methoden u. a. Projekt- und Prozesskontingenzen, die für solche Anlagenprojekte von erheblicher Relevanz sind [88]. Die Berücksichtigung solcher Kontingenzen und weiterer Kostenfaktoren führt zu wesentlich höheren Gestehungskosten im Vergleich zu Peer-Studien, die auf einer vereinfachten Methode basieren und bietet daher eine neue Perspektive auf ebenjene.

Aufgrund dessen, dass eine umfangreiche Analyse unter Berücksichtigung aller drei wichtigen Wasserelektrolysetechnologien durchgeführt worden ist und die Methode vorwiegend nicht zur Berechnung der Gestehungskosten von Wasserstoff und SNG angewendet wird, liefert die Studie eine solide Grundlage für weitere Forschungsarbeiten zu diesem Thema, was den Wert für die wissenschaftliche Gemeinschaft hervorhebt, auch vor dem Hintergrund, dass zukünftige Werte aufgrund der Daten- und Informationslage nicht berechnet werden konnten.

Die Berechnung von Umweltkosten gibt neue Einblicke in den Bereich Umweltkosten von Wasserstoff und SNG, da diese in der Literatur keine Rolle spielen, und bietet daher einen Mehrwert für die Studie und ihre Leser. Darüber hinaus bietet die Berechnung der Umweltkosten eine Grundlage für die Implementierung einer etwaigen Umweltsteuer, sodass deren Berechnung für politische Entscheidungsträger interessant sein könnte. Dies Einführung einer etwaigen Umweltsteuer würde

umweltfreundliche Prozesse fördern und in diesem Zusammenhang gesellschaftliche Schadenskosten, Wohlfahrtsverluste und Treibhausgasemissionen nachhaltig reduzieren.

5.5 Weitere Artikel

Der Autor möchte an dieser Stelle auf die anderen beiden Artikel zu den Gesteungskosten von Wasserstoff und SNG eingehen, die mit der vereinfachten Methode nach Gorre et al. [16] erstellt worden sind. Die Motivation für das Erstellen der Artikel war zum einen, dass sich mit dem Ukrainekrieg und des außergewöhnlichen Anstiegs der Energiepreise ein wichtiger Parameter erheblich verändert hat und zum anderen, dass sich mit der vereinfachten Methode und der Daten- und Informationslage auch zukünftige Werte berechnen lassen konnten. Für die Berechnung der Gesteungskosten sind folgende Szenarien berücksichtigt worden (8000 h, 6000 h, 4000 h Netzenergie und 4000 h Hybrid aus Wind- und Solarenergie). Die Berechnung erfolgte für 10 und 100 MW-Anlagen. Insgesamt sind in den Forschungsartikeln folgende Forschungsfragen beantwortet worden:

1. Welche PtG-Technologie verursacht die geringsten Gesteungskosten für gegenwärtig, 2030 und 2050?
2. Welche Gesteungskosten ergeben sich für grünen Wasserstoff bei einem Preis für elektrische Energie von 20 bis 30 €/MWh und wie lassen sich die Kosten im Vergleich mit blauem und grauem Wasserstoff einordnen?
3. Wie haben sich die Gesteungskosten gegenüber 2021 verändert, nachdem die Großhandelspreise für elektrische Energie in 2022 außergewöhnlich stark gestiegen sind?
4. Wie verändern sich die Gesteungskosten, wenn ein Preis für elektrische Energie von 0 €/MWh angenommen wird?
5. Wie lassen sich die Ergebnisse im Vergleich zu anderen Prozessen, anderen Studien und anderen Preisen einordnen?

Zu den Ergebnissen lässt sich festhalten, dass die SOEC-Technologie, mit Ausnahme des 4000 h-Hybrid Szenarios (gegenwärtig), die geringsten Gesteungskosten für Wasserstoff verursacht, was in Bezug auf SNG für die SOEC-Technologie mit Biomasse als CO₂-Quelle gilt. Wenn die Preise für elektrische Energie für die Produktion von grünem Wasserstoff 20 oder 30 €/MWh betragen, sinken die Gesteungskosten erheblich und liegen zwischen 1,33-2,88 €/kg-H₂ (30 €/MWh) und

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0,95-2,39 €/kg-H₂ (20 €/MWh). Diese Werte sind im Vergleich mit blauem und grauem Wasserstoff wettbewerbsfähig. Im Vergleich zu 2021 haben sich die Gesteuerungskosten von Wasserstoff verdoppelt bzw. fast verdoppelt, während sich die Gesteuerungskosten von SNG für das 10 MW-Szenario um etwa 54 % (4000 h), 77 % (6000 h) und 78 % (8000 h) bzw. für das 100 MW-Szenario um etwa 65 % (4000 h), 86 % (6000 h) und 87 % (8000 h) verändert haben.

Wenn ein Preis für elektrische Energie von 0 €/MWh angenommen wird, sinken die Gesteuerungskosten von Wasserstoff und SNG um etwa 35-99 % (10 MW, H₂) und 45-99,5 % (100 MW, H₂) bzw. um 20-92 % (10 MW, SNG) und 25-95 % (100 MW, SNG), wobei aufgrund der angenommenen Erlöse für Sauerstoff sogar einige negative Gesteuerungskosten für Wasserstoff resultieren. Darüber hinaus stimmen die Ergebnisse für Wasserstoff gut mit den Ergebnissen aus anderen Studien überein und sind bei einem Preis für elektrische Energie von 20 €/MWh wettbewerbsfähig mit konventionellen Verfahren wie *steam methane reforming* und *coal gasification*. Im Vergleich zu Erdgas- und Biogaspreisen liegen die Gesteuerungskosten von SNG nur in Szenarien mit Biomasse als CO₂-Quelle für 2030 und 2050 im Bereich dieser Werte, wenn die Preise für elektrische Energie vollständig berücksichtigt werden. Wird ein Preis von 0 €/MWh angenommen, so liegen alle Werte, bis auf wenige Ausnahmen, im Bereich der Vergleichswerte oder darunter.

6 Fazit und weitere Forschungsarbeiten

Power-to-Gas bietet ein erhebliches Potenzial, um Energie in großen Mengen langfristig zu speichern und kann daher als langfristige Speichertechnologie ein wichtiger Baustein der Energiewende werden. Aus diesem Grund besteht ein erhebliches Interesse an dieser Technologie, weshalb sich diese kumulative Dissertation mit der Lebenszyklus- und techno-ökonomischen Bewertung von PtG-Prozessen in Deutschland beschäftigt hat, um sowohl die ökologische als auch ökonomische Seite dieser Prozesse in die Analyse einzubeziehen, zumal Themen wie Nachhaltigkeit in Zeiten des Klimawandels von steigender Bedeutung sind. Dabei bestand das übergeordnete Ziel der kumulativen Dissertation darin, herauszufinden, welche potenziellen Umweltauswirkungen und Gestehungs- und Umweltkosten bei der Erzeugung von Wasserstoff und SNG in PtG-Prozessen entstehen. Dazu sind verschiedene Elektrolysetechnologien, CO₂-Quellen und Energieszenarien für die Herstellung von Wasserstoff bzw. SNG berücksichtigt worden. Die Arbeit kommt zu folgenden Ergebnissen. Die Produktion von Wasserstoff und SNG ist aus Umweltsichtpunkten für die Szenarien 2019 und 2030 mit der SOEC-Technologie zu empfehlen, während dies für 2050 und das EE-Szenario auf die PEM-Technologie zutrifft. Sofern die aus 100 % EE hergestellten Gase wieder in elektrische Energie umgewandelt werden oder als Kraftstoff für Autos zum Einsatz kommen, ergeben sich im Vergleich zu den berücksichtigten konventionellen Energiequellen und Kraftstoffen z. T. erhebliche Reduktionspotenziale von Treibhausgasemissionen. Dabei verursacht insbesondere grüner Wasserstoff weniger potenzielle Treibhausgasemissionen. Werden die potenziellen Treibhausgasemissionen der Gase mit den CO₂-Emissionen anderer Prozesse verglichen, so sind nur die potenziellen Treibhausgasemissionen des EE-Szenarios niedriger oder im Bereich dieser Vergleichswerte.

Bezüglich der Gestehungskosten von Wasserstoff und SNG kann festgehalten werden, dass sich mit der Methode von Rubin et al. wesentlich höhere Gestehungskosten im Vergleich zu Peer-Studien ergeben, da die Methode detaillierter ist und mehr Kostenfaktoren berücksichtigt. Aufgrund dessen, dass diese Methode vorwiegend nicht für die Berechnung der Gestehungskosten von Wasserstoff und SNG angewendet wird, bieten die Ergebnisse eine neue Perspektive auf ebenjene und darüber hinaus eine Grundlage für weitere Forschungsarbeiten.

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Hinsichtlich der Umweltkosten kann festgehalten werden, dass deren Berechnung eine Basis bietet, um eine etwaige Umweltsteuer einzuführen. Daher könnte die Berechnung der Umweltkosten für politische Entscheidungsträger interessant sein.

Weitere Forschungsarbeiten

Die durchgeführten Arbeiten bieten eine Basis für weitere Forschungsarbeiten. So könnten die erstellten LCA-Modelle mit anderen Energieszenarien kombiniert werden, um so z. B. die potenziellen Umweltauswirkungen von PtG-Prozessen in anderen Ländern zu modellieren. In diesem Zusammenhang besteht auch die Möglichkeit, die potenziellen Umweltauswirkungen nur mit Erneuerbaren zu modellieren. Diesbezüglich könnte man u. a. den direkten Bezug von Wind- und Solarenergie sowie Wasserkraft simulieren und miteinander vergleichen, um herauszufinden, welche regenerative Energiequelle für die Erzeugung von Wasserstoff und SNG die umweltfreundlichste ist. Darüber hinaus bietet es sich an, verschiedene Zeithorizonte zu berücksichtigen, wenn angenommen wird, dass die elektrische Energie aus dem Netz bezogen wird. Denn was passiert, wenn die angenommene Betriebsdauer im EE-Szenario nicht erfüllt werden kann? Welche Auswirkungen hätte in diesem Zusammenhang ein Merit-Order-Effekt, bei dem z. B. Gaskraftwerke, die als essenziell für die Übergangsphase der Energiewende gesehen werden, zugeschaltet werden, um die Nachfrage zu decken? Wie würde sich dies im Vergleich zur Dampfreformierung, der Herstellung von Wasserstoff aus Erdgas, auswirken?

Auch bezüglich der Gestehungskosten gibt es weitere Forschungsmöglichkeiten, da nur gegenwärtige Werte ermittelt werden konnten. Hier könnten bei besserer Datelage und auf Grundlage der durchgeführten Forschungsarbeiten zukünftige Werte für z. B. 2030 oder 2050 ermittelt werden. Darüber hinaus besteht auch die Möglichkeit, dies für andere Länder mit länderspezifischen Parametern durchzuführen, um die Werte in einem internationalen Kontext vergleichen zu können. Dies könnte einen erheblichen Mehrwert für die wissenschaftliche Gemeinschaft liefern. Darüber hinaus könnten auch andere Energieszenarien für die Ermittlung der Gestehungskosten in Erwägung gezogen werden. So ist eine Kombination aus Wind- und Solarenergie für die Berechnung der Gestehungskosten denkbar. Außerdem könnten bezüglich der Umweltkosten weitere Wirkungsindikatoren berücksichtigt werden, um eine detailliertere Berechnung durchzuführen. Zudem könnten

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die Umweltkosten von Wasserstoff und SNG auch für zukünftige Szenarien berechnet werden.

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Rhumspringe, 27. Dezember 2023

Niklas Gerloff

Publikationen

Folgende Publikationen sind für die kumulative Dissertation an der Universität Rostock herangezogen worden, die nachfolgend aufgeführt sind.

Publikation 1: Gerloff N

Comparative Life-Cycle-Assessment analysis of three major water electrolysis technologies while applying various energy scenarios for a greener hydrogen production

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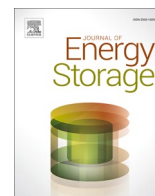
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Abstract: In terms of the decarbonization of industry, transport, electricity generation, and buildings, the production of green hydrogen plays a major role in the strategy of the European Union and Germany. Therefore, the potential environmental impacts of a greener hydrogen production have been analysed taking the three most important water electrolysis technologies alkaline electrolysis (AEC), polymer electrolyte membrane (PEMEC), and solid oxide electrolysis cell (SOEC) into account. To depict a greener hydrogen production, different energy scenarios of Germany –2019, 2030, 2050, and RE (Renewable Energy)– with an increasing share of wind and solar energy have been considered. The study shows how the potential CO₂-eq. of a greener hydrogen production change when applying the different energy scenarios for each technology. On the other hand, the study aims to compare the resulting CO₂-eq. with comparative values of conventional and other hydrogen production processes for classification purposes. Moreover, the study compares the CO₂-eq. results with comparative values of conventional electricity generation and conventional fuels for cars, assuming that the produced hydrogen is used for electricity generation and as a fuel for cars in order to show CO₂ reduction potentials. Besides that, the study compares the Life-Cycle-Impact-Assessment (LCIA) indicators under study to show which technology is potentially the most environmentally friendly one for the respective energy scenario. In summary, it can be stated that the CO₂-eq. decrease with an increasing share of wind and solar energy in the energy mix since the share of fossil energies, which are the main drivers of the CO₂-eq., decline. Furthermore, the SOEC technology has the lowest CO₂-eq. for the energy scenarios in 2019, 2030, and 2050. This applies to the AEC technology for the RE scenario. Regarding the comparative values of conventional and other hydrogen production processes as well as conventional alternatives, only the RE scenario with wind and solar energy provides lower results. Thus, merely the RE scenario is suitable for an environmentally friendly hydrogen production and utilization in order to reduce CO₂ emissions. In addition, the SOEC technology causes the lowest potential environmental impacts for the energy scenarios in 2019 and 2030, taking all LCIA indicators into account. This applies to the PEMEC technology for the energy scenario in 2050 and the RE scenario.



Comparative Life-Cycle-Assessment analysis of three major water electrolysis technologies while applying various energy scenarios for a greener hydrogen production

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ABSTRACT

In terms of the decarbonization of industry, transport, electricity generation, and buildings, the production of green hydrogen plays a major role in the strategy of the European Union and Germany. Therefore, the potential environmental impacts of a greener hydrogen production have been analysed taking the three most important water electrolysis technologies alkaline electrolysis (AEC), polymer electrolyte membrane (PEMEC), and solid oxide electrolysis cell (SOEC) into account. To depict a greener hydrogen production, different energy scenarios of Germany –2019, 2030, 2050, and RE (Renewable Energy)– with an increasing share of wind and solar energy have been considered. The study shows how the potential CO₂-eq. of a greener hydrogen production change when applying the different energy scenarios for each technology. On the other hand, the study aims to compare the resulting CO₂-eq. with comparative values of conventional and other hydrogen production processes for classification purposes. Moreover, the study compares the CO₂-eq. results with comparative values of conventional electricity generation and conventional fuels for cars, assuming that the produced hydrogen is used for electricity generation and as a fuel for cars in order to show CO₂ reduction potentials. Besides that, the study compares the Life-Cycle-Impact-Assessment (LCIA) indicators under study to show which technology is potentially the most environmentally friendly one for the respective energy scenario. In summary, it can be stated that the CO₂-eq. decrease with an increasing share of wind and solar energy in the energy mix since the share of fossil energies, which are the main drivers of the CO₂-eq., decline. Furthermore, the SOEC technology has the lowest CO₂-eq. for the energy scenarios in 2019, 2030, and 2050. This applies to the AEC technology for the RE scenario. Regarding the comparative values of conventional and other hydrogen production processes as well as conventional alternatives, only the RE scenario with wind and solar energy provides lower results. Thus, merely the RE scenario is suitable for an environmentally friendly hydrogen production and utilization in order to reduce CO₂ emissions. In addition, the SOEC technology causes the lowest potential environmental impacts for the energy scenarios in 2019 and 2030, taking all LCIA indicators into account. This applies to the PEMEC technology for the energy scenario in 2050 and the RE scenario.

1. Introduction

To reduce the GHG (Greenhouse Gas) emissions and reach the climate goals, the European Union as well as Germany are working on a hydrogen strategy that shall lead to decarbonization in the sectors of industry, transport, electricity generation, and buildings. Therefore, high investments in the hydrogen infrastructure will be made in the future in order to produce green hydrogen out of renewables, especially from solar and wind energy. Moreover, green hydrogen has the potential to be the climate-friendly mineral oil of tomorrow and can help mitigate climate change [1,2]. With a share of more than 90%, the oil and

ammonium production industries are the main users of hydrogen [3,4]. Also, hydrogen can be used to stabilize the electricity grid if fluctuations occur due to the expansion of renewables, especially by wind and solar energy [5]. Moreover, hydrogen is a promising fuel for vehicles since the combustion of H₂ is pollutant-free, and cars driven by hydrogen have a longer range in comparison to electric cars [6–8]. The amount of hydrogen produced in Germany is around 19 billion Nm³ per year, where only 5% is produced by electrolysis [9]. Most of the hydrogen is produced by fossil fuels, such as natural gas, heavy oils, or coal, contributing to approx. 19 Mio. t CO₂ emissions per year [9] which makes a greener hydrogen production with a reduction of CO₂ emissions impossible [5,10].

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Abbreviations		Chemical sum formula	
AE	Accumulated Exceedance	CO ₂	Carbon dioxide
AEC	Alkaline-Electrolysis	e ⁻	Electron
APOS	Allocation at Point of Substitution	H ₂	Hydrogen
BDLR	Biomass derived liquid reforming	H ₂ O	Water
BoP	Balance-of-Plant	H ₃ O ⁺ /H ⁺	Oxonium ion
CG	Coal gasification	KOH	Potassium hydroxide
CNG	Compressed Natural Gas	O ²⁻	Oxide ion
DE	Represents Germany in the ecoinvent database	OH ⁻	Hydroxide ion
DF-MEC	Dark fermentation-microbial electrolysis cell	Y ₂ O ₃	Yttrium oxide
DNA	Deoxyribonucleic acid	ZrO ₂	Zirconium oxide
ENTSO-E	European Network of Transmission System Operator	<i>Units of LCIA indicators</i>	
Eq.	Equation	CFC-11-eq.	Trichlorofluoromethane equivalent, unit of ozone layer depletion
Fig.	Figure	CO ₂ -eq.	Carbon dioxide equivalent, unit of Global Warming Potential
FU	Functional unit	CTUh	Comparative Toxic Unit for humans, unit of carcinogenic effects
GHG	Greenhouse Gas	Mol H ⁺ -eq.	Unit of acidification potential
GLO	Represents global in the ecoinvent database	NMVOC-eq.	Non-Methane Volatile Organic Compounds equivalents, unit of photochemical ozone creation
GWP	Global Warming Potential	P-eq.	Phosphor equivalent, unit of freshwater eutrophication
ILCD	International Life Cycle Data	PM2.5	Particulate Matter less than 2.5 micrometre
IndWEDe	Industrialisierung der Wasserelektrolyse in Deutschland	U ²³⁵ -eq.	Uranium-235 equivalent, unit of ionizing radiation
IPCC	Intergovernmental Panel on Climate Change	<i>Units</i>	
ISO	International Organization for Standardization	A/cm ²	Ampere per square metre
LCA	Life-Cycle-Assessment	ft	Foot
LCI	Life-Cycle-Inventory	g	gram
LCIA	Life-Cycle-Impact-Assessment	h	Hour
LHV	Lower Heating Value	kg	Kilogram
LPG	Liquefied Petroleum Gas	km	kilometre
LSM	Lanthanum-Strontium-Manganite	kW	Kilowatt
MEA	Membrane Electrode Assembly	kWh	Kilowatt hour
ODP	Ozone Depletion Potential	l	Litre
PEMEC	Polymer-Electrolyte-Membrane -Electrolysis-Cell	m ³ _{H2}	Cubic metre of hydrogen
PEMFC	Polymer-Electrolyte-Membrane-Fuel- Cell	MJ	Megajoule
PV	Photovoltaic	MW	Megawatt
RE	Renewable Energy	Nm ³	Standard cubic metre
RER	Represents Europe in the ecoinvent database	t	Ton
RoW	Represents Rest-of-the-World in the ecoinvent database	TWh	Terawatt hour
SI	Supplementary Information	USD	US-Dollar
SMR	Steam methane reforming	°C	Degrees Celsius
SOEC	Solid-Oxide-Electrolyzer-Cell		
SOFC	Solid-Oxide-Fuel- Cell		
Tab.	Table		
U.S.	United States		
UVB	Ultraviolet-B rays		
w/w	Weight per weight		
wt. %	Weight percent		

Since the hydrogen production in Germany is directly correlated to high CO₂ emissions, the study aims to examine a greener hydrogen production by water electrolysis in order to analyse the potential environmental impacts –in particular the CO₂-eq.– of said greener produced hydrogen. For this purpose, the most important water electrolysis technologies –AEC, PEMEC, and SOEC for a system size of 1 MW– have been considered. Moreover, various energy scenarios of Germany –2019, 2030, 2050, and RE– with an increasing share of wind and solar energy have been taken into account in order to depict a greener hydrogen production.

Because the GWP (Global Warming Potential) is the most important indicator [5], the resulting CO₂-eq. are analysed in more detail and compared with conventional and other hydrogen production processes. Besides that, the greener produced hydrogen is assumed to be used for electricity generation or as a fuel for cars. Thus, the results can be

compared to conventional alternatives in order to show a CO₂ reduction potential which can help to achieve the climate goals and mitigate climate change. In addition, which technology is potentially the most environmentally friendly one for the respective energy scenario is also analysed in this study, considering more indicators than only the GWP. In total, the following research questions will be answered in this paper.

1. How do the CO₂-eq. results change regarding an increasing share of wind and solar energy in the energy mix, and which technology shows the lowest CO₂-eq.?
2. How do the CO₂-eq. differ in comparison to conventional and other hydrogen production processes?
3. How do the CO₂-eq. results of the greener produced hydrogen differ in comparison to conventional alternatives, assuming that the produced hydrogen is used for electricity generation or as a fuel for cars?

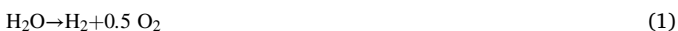
Table 1
Cathode and Anode reaction of the different water electrolysis technologies (Eq. 2-7).

	AEC	PEMEC	SOEC
Cathode reaction	$2\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + 2\text{OH}^-$	$2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$	$\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + \text{O}^{2-}$
Anode reaction	$2\text{OH}^- \rightarrow \text{H}_2\text{O} + 0.5 \text{O}_2 + 2\text{e}^-$	$\text{H}_2\text{O} \rightarrow 2\text{H}^+ + 0.5 \text{O}_2 + 2\text{e}^-$	$\text{O}^{2-} \rightarrow 0.5 \text{O}_2 + 2\text{e}^-$

4. Which water electrolysis technology is potentially the most environmentally friendly one for each scenario taking all indicators into account?

1.1. Water electrolysis

Water electrolysis describes the process of splitting H_2O (Eq. (1)) into its basic components hydrogen and oxygen. This happens at the anode and cathode of the electrolyzer, where hydrogen is formed at the negatively charged cathode, and oxygen is formed at the positively charged anode (see Eq. (2)–(7) in Table 1) [11].



The three water electrolysis technologies have different charge carriers $-\text{OH}^-$ (AEC), $\text{H}_3\text{O}^+/\text{H}^+$ (PEMEC), O^{2-} (SOEC). These are further illustrated in Section 2.2.

1.2. Life-Cycle-Assessment (LCA)

What is Life-Cycle-Assessment? Concerning the ISO norms 14040 and 14044, LCA is an environmental management tool which examines potential environmental impacts between a technical system (technosphere) and the environment. For this, inputs and outputs of products, plants, and services are considered, for example, from cradle (raw material extraction) to grave (final disposal) [12,13].

Consequently, LCA can be helpful in various ways, for example, as information for decision-makers and improvements of manufacturing processes of products. A LCA study comprises of 4 phases according to ISO 14040 and 14044 [12,13]:

1. The goal and scope definition phase include the goal, the system boundary, and the functional unit (FU) of the study etc.
2. The inventory analysis phase covers the input and output data which are necessary to implement the LCA.
3. The impact assessment phase comprises additional information for a better understanding of the environmental impacts of the life cycle data.
4. The interpretation phase includes the evaluation of the results as well as the conclusions and recommendations regarding the goal of a LCA study.

1.3. Previous studies

There are a few studies relating to the topic of Life-Cycle-Assessment of hydrogen production [5,14–19] which are mostly focused on the GWP only and hardly address other impact indicators, such as eutrophication or the ozone depletion potential (ODP) [5,19]. This is especially represented by Bhandari et al. [14] who analysed 21 LCA studies. Moreover, there is no study present, to the knowledge of the author, that carried out a detailed LCA taking more indicators than the GWP into account on the three most important water electrolysis technologies considering different energy scenarios with an increasing share of wind and solar energy for a greener hydrogen production to show which technology is potentially the most environmentally friendly one for each scenario. Furthermore, the comparison of the CO_2 -eq. of the greener produced hydrogen with CO_2 emissions of conventional alternatives, under the assumption that the produced hydrogen is used to generate electricity or

as fuel for cars, to show a reduction potential of the CO_2 emissions holds novelty as well [5,14–19]. Hence, the study aims to fill the research gaps and show which water electrolysis technology is potentially the most environmentally friendly one regarding the respective energy scenario. Moreover, this study aims to show the CO_2 reduction potential of greener produced hydrogen compared to conventional alternatives, assuming that the produced hydrogen is used for electricity generation or as a fuel for cars.

Because the GWP is the most important indicator, the GWP results are compared with values of other LCA studies and conventional hydrogen production processes (see Section 3), even though a comparison with other LCA results is limited [18]. For this, the following GWP values have been considered from other LCA studies for the comparison in Section 3. For the AEC technology, the value published by Zhang et al. [17], which is approx. 275 g of CO_2 -eq./MJ using the ENTSO-E supply (which stands for the European Network of Transmission System Operators), has been considered, while the value of 29.5 kg CO_2 -eq./kg H_2 has been taken into account according to Bareiß et al. [5] for the PEMEC technology, and the value of 28.85 kg CO_2 -eq./kg H_2 has been taken into consideration according to Mehmeti et al. [18] for the SOEC technology.

2. Methodology

The methodology can be divided into two sections. The section “Scope of the LCA study” and the section “Water electrolysis technologies and generation of the LCI (Life-Cycle-Inventory) data”. In the first section, the scope of the study is illustrated, while in the second section, the water electrolysis technologies and the data generation are discussed and described.

2.1. Scope of the LCA study

In this chapter, the scope of the LCA study is described. The scope includes the system boundary, the assumed lifetime of the BoP (Balance of Plants) and stack components, the functional unit of the process, the different scaling factors, and the estimation of the additional manufacturing energy. Furthermore, the various energy scenarios, the produced amount of hydrogen during the estimated lifetime, the operating data, the chosen disposal and treatment processes of the materials, and the selected Life-Cycle-Impact-Assessment indicators are described in this chapter as well.

This study aims to avoid complex allocation as recommended by ISO 14044 [13]. Therefore, the allocation cut-off method has been chosen as the system model of the LCA study from cradle to grave, assuming that the hydrogen production process is a single output process, and the produced oxygen is released into the atmosphere. The allocation at point of substitution (APOS) method, normally used for multi-output processes, is, therefore, not suitable for this study. The consequential method, that is used for long-term future scenarios, is also not suitable for the LCA study due to higher uncertainties [20].

Besides this, the geographical reference Europe has been selected for the processes. If no processes with the geographical reference of Europe were available, processes with the geographic reference RoW (Rest of the World) or GLO (Global) have been chosen. Further, Germany (DE) has been chosen provided that the opportunity for it existed.

In addition, two transport ways of the components have been assumed. The first transport way relates to the manufacturing process

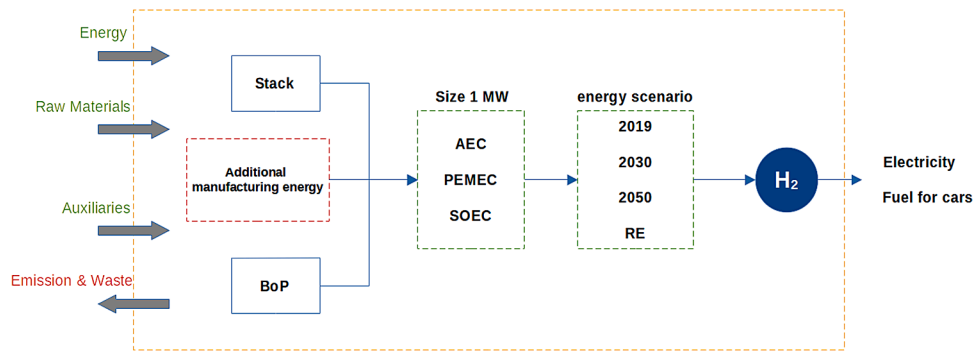


Fig. 1. System boundary.

including the transports for assembly purposes and the delivery of single items. The second transport way includes the transport distance of the components to the location of the water electrolysis plant. It is assumed that the length of each transport way is 250 km for every component.

The weight of the components times 250 km divided by the produced amount of hydrogen in 20 years (see Section 2.1.7) leads to the result in metric ton*km/kg H₂ entered in the software. To model the transport phase, transportation with freight lorry > 32 t, Euro 6 [RER], has been chosen [21].

Moreover, additional manufacturing energy of stack and BoP components has been estimated since theecoinvent processes do not always cover the total manufacturing energy of these components [21] (see Section 2.1.5).

2.1.1. System boundary

The system boundary of the LCA study (see Fig. 1) consists of the stack and BoP components of the 1 MW water electrolysis technologies and the different energy scenarios. Moreover, additional manufacturing energy has been added. The processes for energy, raw materials, and auxiliaries originate from theecoinvent database version 3.5 [21].

2.1.2. Lifetime of water electrolysis plants

A lifetime of 20 years, operating 8000 h per year, has been assumed for the components of the electrolysis technologies without considering the stack components [22]. According to a study called IndWEDe [23], it is assumed that the stacks are replaced 3 times during the 20 years lifespan, based on the 2030's scenario for 1 MW systems which predicts a lifetime of 50,000 h or more for the stacks of the different water electrolysis technologies.

2.1.3. Functional unit

According to ISO 14040, a functional unit needs to be scalable and satisfy a function [12]. Since hydrogen can be used in various ways, the function is to generate electricity or to drive a car as a fuel, while the reference flow of the systems corresponds to 1 kg H₂ to make the FU

scalable. Furthermore, the weights of the components have been divided by the assumed, produced amount of H₂ in 20 years (see Section 2.1.7) in order to obtain the values relating to the FU of 1 kg H₂. The values of the stack components have been multiplied with a factor of 3 since 3 stack replacements are assumed during the lifetime (see above).

2.1.4. Scaling factors

Some BoP and stack components had to be scaled up or down to get data for the 1 MW systems. Therefore, the scaling method according to Remer and Chai [24] has been applied in this study and modified according to Zhang et al. [25], as shown in the following equation:

$$\frac{C_2}{C_1} = \left(\frac{X_2}{X_1}\right)^b \tag{8}$$

- C₁ – known weight of component 1
- C₂ – unknown weight of component 2
- X₁ – capacity (e.g., volume or mass flow) of plant, equipment, or component 1
- X₂ – capacity (e.g., volume or mass flow) of plant, equipment, or component 2
- b – scaling factor

The scaling method has been modified to estimate the weight of single components due to lack of information. For example, to be able to estimate the weight of the same component that is used for different mass or volume flows, the weight of this component has been scaled up or down with the corresponding mass or volume flows. Furthermore, the scaling factor of 0.7 for BoP components has been selected according to [25].

The scaling factor of 0.88 [26] has been chosen for stack components because it is assumed that the material use and the manufacturing energy of the stacks do not increase linearly with the plant sizes. This deviates from the approach of Zhang et al. and Mehmeti et al. [17,18] since both assume a linear increase. To proof that this scaling factor is appropriate, the following calculation has been done (see Table 2 and Eq. (9)) [27,28].

$$c_2 = \left(\frac{7130 \text{ kW}}{1 \text{ kW}}\right)^{0.88} * 280 \text{ kWh} = 688,457 \text{ kWh} \tag{9}$$

According to Häfele et al. [28], 280 kWh are needed for the manufacturing and assembling of a 1 kW SOEC stack, while independently of that the manufacturing and assembling energy of a 7.13 MW

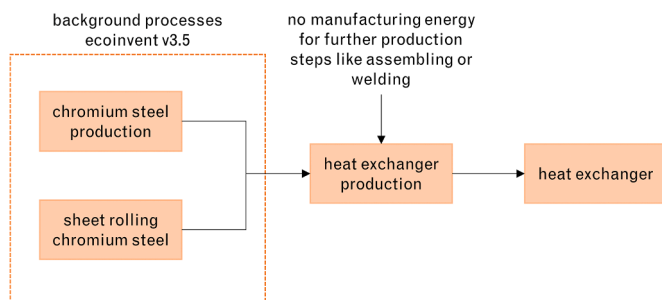


Fig. 2. Heat exchanger production (schematic).

Table 2 Proof of scaling factor 0.88 (values from [27,28]).

Size in kW	Manufacturing energy in kWh
1	280
7,130	695,000

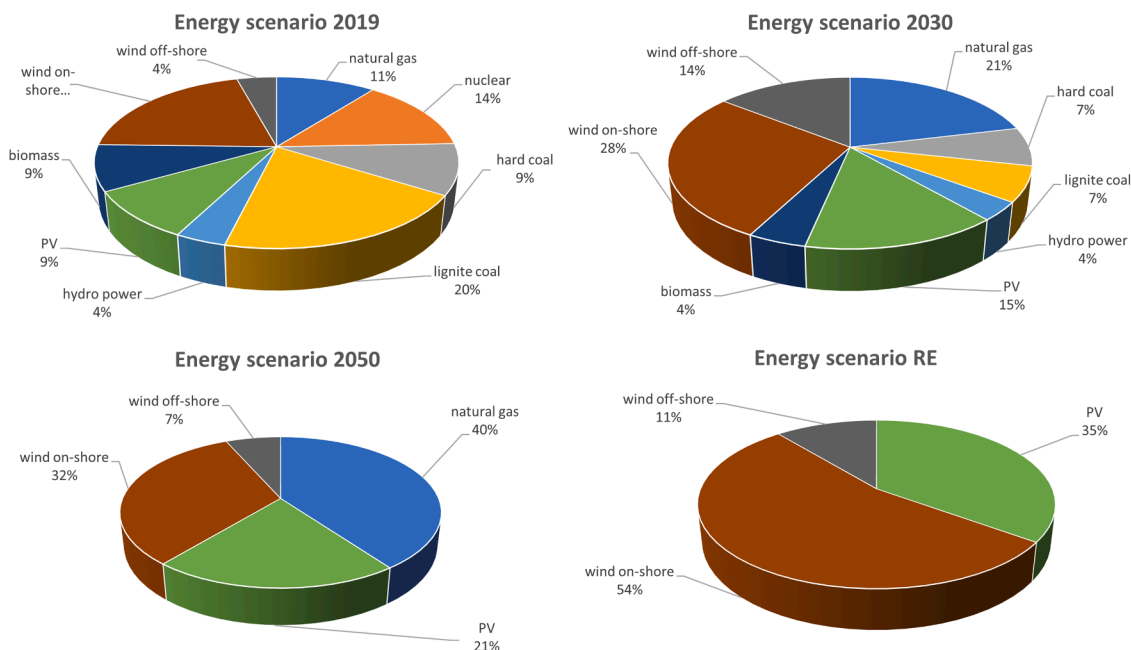


Fig. 3. Energy scenarios.

SOEC stack is 695,000 kWh in accordance with Patyk et al. [27]. An up-scaling from 1 kW to 7.13 MW with the stated energy of 280 kWh and a scaling factor of 0.88 leads to a result of approx. 688,457 kWh. That is in the range of the specified amount of energy according to Patyk et al. [27]. Thus, the scaling factor of 0.88 is appropriate, while the linear scaling method according to Zhang et al. and Mehmeti et al. is less compatible and leads to a result almost 3 times higher than the value published by Patyk et al.

2.1.5. Estimation of manufacturing energy

Since the total manufacturing energy of components is hardly covered by ecoinvent processes, an estimation of the manufacturing energy for these components has been carried out. Fig. 2 shows the example of a heat exchanger production.

To constitute the production process of a heat exchanger, the ecoinvent processes chromium steel production and sheet rolling chromium steel have been selected in accordance with [29]. These processes only include the manufacturing energy of the raw material chromium steel, while the manufacturing energy of further production steps, such as assembling or welding, is not considered. Thus, additional manufacturing energy has been added according to literature. The values of the additional manufacturing energy are briefly discussed in the SI Section 1.

(in kWh/kg H ₂)	51.8	54	42.3	: 11.2 Nm ³ H ₂ /kg H ₂
	↓			
	AEC	PEMEC	SOEC	
Size in kW	4.63	4.82	3.78	kWh/Nm ³ of H ₂
1000	216.0	207.5	264.6	
	↓			
	Nm ³ of H ₂ /h		x 0.0893 kg/Nm ³ of H ₂	
	AEC	PEMEC	SOEC	
kg of H ₂ /h	19.3	18.5	23.6	
	↓			
	x 8000 h		x 20 years	
	AEC	PEMEC	SOEC	
kg of H ₂ in 20 years	3,085,961	2,964,315	3,779,894	

Fig. 4. The produced amount of hydrogen in 20 years.

2.1.6. Energy scenarios

In order to constitute a greener hydrogen production, the energy scenarios in 2019, 2030, 2050, and the RE scenario have been considered. The composition of the energy scenarios is shown in Fig. 3. The values stem from [5,30,31].

For the energy scenario in 2030, the value of 619 TWh (net electricity generation) published by Aurora Energy Research has been considered. The electricity generation from oil (1 TWh) was neglected because the overall share is just 0.16%. Moreover, the other energy sources (27 TWh), which are not specialized by Aurora Energy Research, have not been taken into account. Thus, the 28 TWh have been subtracted, leading to a total amount of 591 TWh. The percentage values of the listed energy scenario in 2030 (see Fig. 3) result after the values of the listed energy sources [31] have been set in relation to the value of 591 TWh. The values for the energy scenarios in 2050 and the RE scenario come from Bareiß et al. [5] who created energy models computationally to forecast future energy scenarios for Germany. The only distinction regarding the values by Bareiß et al. –as well as for the scenarios in 2019 and 2030– is that the values for wind energy have been divided into wind on- and offshore parts according to data released by Aurora Energy Research for the year 2017 in order to draw a more realistic picture of the energy mixes. Therefore, the following calculation has been conducted: The total wind energy produced in 2017 was around 106 TWh, of which 88 TWh were produced by onshore and 18 TWh by offshore windmills according to [31]. Thus, 83% (88 TWh divided by 106 TWh) of the total wind energy were produced by onshore and 17% (18 TWh

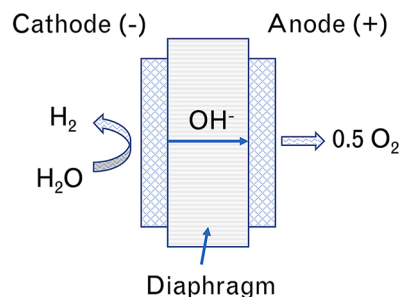


Fig. 5. Working principle of AEC technology.

Table 3
Operating data.

Operating data per kg H ₂	Water demand H ₂ production (l) ¹	Water demand cooling & compressor (l) ²	Electricity demand (kWh) ³	KOH (kg) ⁴	Heat (kWh) ⁵
AEC	8.9	88.1	51.8	0.0037	-
PEMEC	8.9	88.1	54	-	0.28
SOEC	8.9	644.7	42.3	-	5.24

divided by 106 TWh) by offshore windmills. The results of 83% and 17% have been considered for every energy scenario in order to divide the total wind energy into on- and offshore parts, assuming that these shares do not change in the future.

The estimated manufacturing energy (see SI Section 1) and the operating energy (Table 3) have been multiplied with the percentage values in Table 3. These values have been entered in Umberto+.

2.1.7. Produced amount of H₂

In this part, an estimation of the produced amount of hydrogen during the 20 years lifetime is carried out. The starting point of the calculation is the assumption that the production of 1 kg hydrogen requires 51.8 kWh (AEC), 54 kWh (PEMEC), and 42.3 kWh (SOEC) based on the specific energy requirement taken from the IndWEde study [23]. In the IndWEde study, three values of the specific energy requirement in kWh/kg H₂ are given for each technology (progressive, central, and conservative). Therefore, the average values have been calculated. In the next step, these values have been divided by 11.2 Nm³ H₂/kg H₂ [29] to obtain the values in kWh/Nm³ H₂. Furthermore, the system size of 1 MW has been divided by these values to get the results in Nm³ H₂ per hour. Next, to receive the results in kg H₂ per h, the results have been multiplied with the density of H₂ under normal condition (1 bar, 15 °C) [29]. Subsequently, the values have been multiplied with the operating hour of 8000 h/year and the lifetime of 20 years, as shown in Fig. 4.

Note that a 100% yield is assumed. Therefore, no conversion losses have been considered in the calculation.

2.1.8. Operating data

Table 3 illustrates the operating data for all technologies. Further explanations (superscript numbers) can be found in the SI Section 2.

2.1.9. Disposal and treatment of materials

Because there are hardly any recycling processes for the disposal phase as well as only limited waste treatment and disposal processes for materials available in the database, the following processes (see Table 4) have been selected to model the disposal phase.

2.1.10. LCIA factors

There are several options of LCIA methods in Umberto+, of which most are obsolete [32]. Therefore, the latest LCIA method in Umberto+, ILCD 2.0 midpoint 2018, has been selected with one exception. The IPCC 2013 method has been applied for the GWP. The selection of the impact indicators –shown below in Table 5– is based on the levels of recommendations of the International Life Cycle Data system (ILCD). Only impact indicators with either level I (recommended and satisfactory) or level II (recommended but in need of some improvements) have been chosen [33].

2.2. Water electrolysis technologies and generation of the LCI data

In this paragraph, the working principles of the different water electrolysis technologies are briefly discussed. Moreover, the LCI data generation and origin of the data are described. Due to the large amount of data, only the component names are listed in the tables. Values for these components as well as the corresponding ecoinvent processes can be found in the SI Figs. 1-4.

2.2.1. Alkaline electrolysis (AEC)

Alkaline water electrolysis is the most developed, mature, and commercially available technology since decades [34]. The electrolyte –potassium hydroxide (KOH) 20–40 wt.%– is highly corrosive which leads to high maintenance costs [35].

The technology is available for large plant sizes and operates with a stack efficiency of up to 67 % (based on the lower heating value (LHV) of the generated H₂) [36]. The operating temperature is in between 60–80 °C, and the current density is around 0.2–0.4 A/cm² [37]. Moreover, the system energy –including the stack and periphery energy– is in the range of 4.4–6.6 kWh/m³H₂, while the gas purity is higher than 99.5%, and the operating pressure is below 30 bar [37–39]. The stack lifetime is in between 60.000 to 90.000 h [37]. The following figure (Fig. 5) shows the schematic working principle of the electrolyzer.

As mentioned above, hydrogen is formed at the cathode, and oxygen is formed at the anode. The charge carrier OH⁻ moves from the cathode to the anode through the diaphragm.

Generation of LCI data

The BoP and stack components of the AEC technology are shown in Table 6. While the LCI data of the BoP components either originate from Zhang et al. [29], based on a 300-kW system and, therefore, scaled-up to 1 MW by a factor of 0.7, the LCI data of the other BoP components originate from manufacturer offers [40,41] or have been estimated by own calculations using additional information by the producers [42,43,44].

In addition, the stack components data (19,20) are derived from Zhang et al. [29], while the diaphragm component (Zirfon) originate from Huebner [45]. Since there is no given production process of Zirfon in the ecoinvent database, the processes polysulfone production and zirconium dioxide production have been chosen to constitute the production of Zirfon. The weight of the diaphragm has been divided into 40% polysulfone and 60% zirconium dioxide according to Agfa company [46]. All stack components values are based on a 300-kW system; therefore, these values have been scaled to 1 MW by a factor of 0.88 (see Section 2.1.4).

2.2.2. Polymer electrolyte membrane (PEMEC)

In comparison to AEC electrolyzers, PEMEC electrolyzers are less mature. However, the electrolyzers have evolved since the first drafts by General Electric 55 years ago [47]. Moreover, PEMEC electrolyzers are more expensive due to the use of noble catalysts, such as platinum and iridium [36]. For the future, a decline of investment costs is expected, making the electrolyzers more attractive from an economic point of view [35,37]. As shown in Fig. 6, the membrane electrode assembly (MEA) is connected with the anode and the cathode and separates both. Thus, the charge carrier H⁺ can move from the positively charged anode –where oxygen is formed– to the negatively charged cathode –where hydrogen is formed–.

Furthermore, the PEMEC technology is commercially available and operates with a similar system efficiency as the AEC technology. However, the current density and the gas purity are higher with values in between 0.6–2.0 A/cm² and > 99.99%, respectively [37]. Besides this, the operating pressure (below 200 bar) is significantly higher in comparison to AEC systems, while the operating temperature (50 °C to 80 °C) and the system energy (4.2–6.6 kWh/m³H₂) are similar to AEC systems [37–39].

Generation of LCI data

Table 4

Disposal phase processes.

Overview of selected disposal processes from the ecoinvent database v.3.5

market for scrap steel [Europe without CH]	market for scrap copper [Europe without CH]
treatment of waste reinforcement steel, sorting plant [RoW]	market for waste plastic, mixture [DE]
market for scrap aluminium [Europe without CH]	treatment of waste zeolite, inert material landfill [RoW]
market for waste plastic, industrial electronics [RoW]	market for waste rubber, unspecified [Europe without CH]
treatment of used cable [GLO]"	treatment of waste concrete, not reinforced, sorting plant [Europe without CH]
treatment of scrap printed wiring boards, shredding and separation [RoW]	treatment of waste bulk iron, excluding reinforcement, sorting plant [Europe without CH]
treatment of waste polyethylene/polypropylene product, collection for final disposal [Europe without CH]	

The PEMEC BoP and stack components data (see Table 7) stem from Bareiß et al. [5] and correspond to a 1 MW system. Moreover, some further BoP components like water purifier & feed tank, buffer tank, and heat exchanger have been added, derived from a 300 kW AEC system [29], under the assumption that the components are also suitable for a PEMEC system. The values have been scaled up from 300 kW to 1 MW.

With respect to the stack components, two materials are not present in the database. Firstly, there is no process for Nafion in the ecoinvent database available. Instead, the process of tetrafluoroethylene production has been selected [48]. Secondly, iridium is not listed in the database as well. Consequently, data of a study published by the Federal Environment Agency of Germany have been used to depict the production of iridium and the associated potential environmental impacts [49]. Moreover, the data from the study have been adjusted; thus, they relate to 1 kg of iridium.

2.2.3. Solid oxide electrolysis cell (SOEC)

The SOEC technology is the least evolved technology and needs some further research to be commercially available [37,47]. The technology operates at temperatures between 650 °C and 1000 °C using solid ion-conducting ceramics –mostly zirconium oxide (ZrO₂) with yttria oxide (Y₂O₃)– for the electrolyte [37,50–52]. The charge carrier O²⁻ passes through the ion-conductor from the cathode to the anode and reacts with oxygen, as shown in Fig. 7 [35].

Besides that, the technology operates with an operating pressure of below 25 bar as well as a gas purity of around 99.9%. Moreover, the current density is in the range of 0.3–2.0 A/cm², and the system energy is >3.7 kWh/m³H₂ [37,50]. The main challenges for the SOEC technology are, on the one hand, long term stability of the system and, on the other hand, material degradation concerning high-temperature operation [53].

Generation of LCI data

Since this technology is immature, the data collection regarding SOEC stack and BoP components was difficult. Nevertheless, the BoP and stack data, listed in Table 8, have been collected and estimated using data by manufacturer offers, Zhang et al., and Patyk et al. [29,54]. Patyk et al. analysed a 7.13 MW SOEC system that includes 11 heat exchangers and 5 hydrogen compressors [27,54]. While the values for the 5 hydrogen compressors stem from Zhang et al. [29] and have been assumed for 1 MW systems, the data for the heat exchangers [54], that stem from Patyk et al. [54], have been scaled down accordingly to 1 MW.

Further BoP components, such as mixer, splitter, heater for pre-heating, water pump, and separator, are based on manufacturer information or own calculations [55–60]. Furthermore, it has been assumed that the control panels of the heaters and the frequency converter of the water pump consist of the same materials as in Zhang et al. [29] since no further specification have been made by the manufacturers. These values have been allocated proportionately regarding the weight. Moreover, additional BoP components, such as water purifier & feed tank and a buffer tank, have been added in accordance with Zhang et al. [29]. These components have been scaled up differently based on the water requirements per h and the hydrogen production rate per h since these parameters differ significantly from the 1 MW AEC and PEMEC systems. Therefore, the explained method above, scaling from 300-kW to 1 MW, could not be applied.

Because the calculation of pipes and tubing is very difficult corresponding to the expert opinion of Mr. Koester (ThyssenKrupp) [61], the same tubing as for a 100 kW Solid-Oxide-Fuel-Cell (SOFC, 300 kg) [62] has been assumed and scaled up to 1 MW with a scaling factor of 0.7.

The SOEC stack data are based on Häfele et al. [28]. These data refer to a 1 kW stack and have been scaled up to 1 MW using a scaling factor of 0.88. Since there are no given data for stack the materials yttrium, lanthanum strontium manganite (LSM), and glass sealant paste in the ecoinvent database, assumptions had to be made. Thus, yttrium has been replaced by "samarium europium gadolinium concentrate, 94% rare

Table 5
Impact categories and impact factors.

Nr.	Impact category	Impact indicator	Abbreviation	Level
1	Human health	Ozone Depletion Potential (Ozone layer depletion)	ODP	I
2	Human health	Carcinogenic effects	CE	II
3	Human health	Particulate matter (respiratory effects)	PM	I
4	Human health	Ionizing radiation	IR	II
5	Human health	Photochemical ozone creation	POC	II
6	Ecosystem quality	Freshwater & terrestrial acidification	Acid.	II
7	Ecosystem quality	Freshwater eutrophication	Eutr.	II
8	Climate change	Global Warming Potential (GWP 100)	GWP	I

earth oxide". Further, the production of LSM and its ingredients is based on Staffell et al. [63] and the periodic table. For the glass sealant paste, data from the Schott AG have been considered [64]. The composition of the glass sealant paste consists of aluminium -, boron-, barium-, and silicon oxide, whereas silicon oxide is not available in the database.

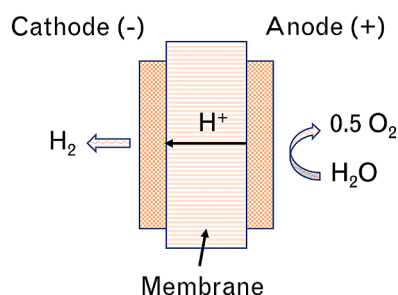


Fig. 6. Working principle of PEMEC technology.

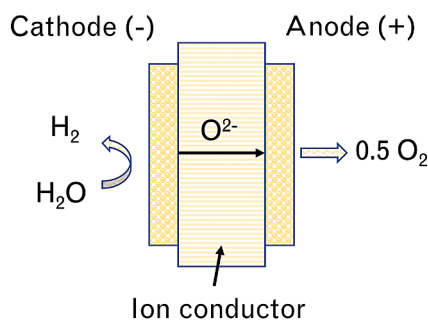


Fig. 7. Working principle of SOEC technology.

Table 6
AEC stack and BoP components.

AEC: Stack and BoP components [5,29,40–45, *]			
BoP components			
1	Water purifier & feed tank	12	Heat exchanger
2	Control panel/electronics	13	Gas separator (2 x)
3	Transformer and rectifier	14	Alkali-resistant rotary pump
4	Hydrogen dryer and deoxidizer	15	Steel tank for KOH
5	Frequency converter diaphragm compressor	16	Storage tank
6	Diaphragm, for diaphragm compressor	17	Container
7	Container with pipes and fittings for diaphragm compressor	18	Foundation (concrete)
8	Buffer tank		Stack components
9	Tubing and cables	19	Anode and cathode with frame
10	Water cooling plant for electrolyzer	20	Gasket
11	Pumps and coolers	21	Diaphragm, zirfon
KOH = potassium hydroxide; * own calculations/assumptions			

Therefore, the process for pure silicon has been selected, assuming that similar potential environmental impacts occur. Lime with < 1% w/w has been neglected [64]. The allocation has been assumed with 25% each because the composition of the single materials varies between 10–50% w/w [64]. Moreover, the process market for heat, district or industrial which consists of about 52% heat from coal and peat, 16% heat from oil, 18% heat from biofuels (modelled with biogas and wood), 11% heat from waste, and 2% heat from other sources [21] has been chosen because it is assumed that the heat is supplied by an external source to convert water into steam, as recommended by [65].

2.2.4. General assumptions of single components

General assumptions of single components are described in Section 3 in the SI.

3. Results and discussion

In this section, the LCIA results are discussed, and the research questions mentioned at the beginning will be answered. In part 3.1, the GWP results are analysed in more detail and classified considering comparative values. Therefore, in 3.1.1, the GWP results are compared with results from other LCA studies and other hydrogen production processes, while in 3.1.2, the GWP results are compared with CO₂ emissions of conventional fuels for cars and conventional electricity generation. Section 3.2 comprises the LCIA results. In part 3.2.1, the maximum values of the LCIA results are presented which have been used to scale the relative LCIA results in Fig. 12. In addition, the LCIA results (except the GWP) are described, and the change in the results regarding the energy scenarios are discussed in part 3.2.2. Moreover, the LCIA results are compared with one another in part 3.2.3 to show which technology is potentially the most environmentally friendly one for each scenario.

3.1. GWP results

The GWP of the water electrolysis technologies decreases by more

Table 8
SOEC stack and BoP components.

SOEC: Stack and BoP components [5,28,29,43,54-60,61, *]			
	BoP components		
1	Heat exchanger (11)	13	Water purifier & feed tank
2	Frequency converter diaphragm compressor (5)	14	Buffer tank
3	Diaphragm, for diaphragm compressor (5)	15	Container
4	Container with pipes and fittings for diaphragm compressor (5)	16	Foundation (concrete)
5	Power electronics (rectifier, voltage adaption)	17	Tubing
6	Control electronics		Stack components
7	Mixer (2)	18	Air electrode
8	Splitter (2)	19	Glass sealant
9	Heater (gas-preheating)	20	Blocking layer
10	Heater (water)	21	Interconnect (including LSM layer)
11	Separator	22	Electrolyte
12	Water pump	23	H ₂ -electrode (including nickel mesh)
	LSM = Lanthanum Strontium Manganite; * own calculations/assumptions		

than 21% from 2019 to 2030. Moreover, the CO₂-eq. decline by more than 14% from 2030 to 2050 as well as by more than 75% from 2050 to the RE scenario (see Fig. 8).

Since lignite coal is the main driver of the CO₂-eq. in the energy scenario in 2019 with a share of 19.8%, the reduction from 19.8% to 6.6% in 2030 (see Fig. 3) and to 0% both in 2050 and the RE scenario is one of the main reasons for the decrease of the CO₂-eq. Besides this, the decline of hard coal as the second main driver of the CO₂-eq. in 2019's energy scenario from 9.5% to 7.3% in 2030 and to 0% both in 2050 and the RE scenario is another main reason for the decrease of the CO₂-eq.

Because natural gas as the main contributor to the 2050's CO₂-eq. results is not present in the RE scenario anymore, the CO₂-eq. decrease sharply when applying the RE scenario. In total, the CO₂-eq. sink with fewer fossil fuels and higher shares of wind and solar energy in the energy mix. Moreover, the PEMEC technology shows the highest CO₂-eq. of the energy scenarios in 2019, 2030, and 2050, whereas the SOEC technology shows the lowest results concerning these scenarios. Further, the maximum value of the RE scenario refers to the 1 MW SOEC plant, mostly due to the heat demand for the hydrogen production, while the minimum value refers to the 1 MW AEC plant.

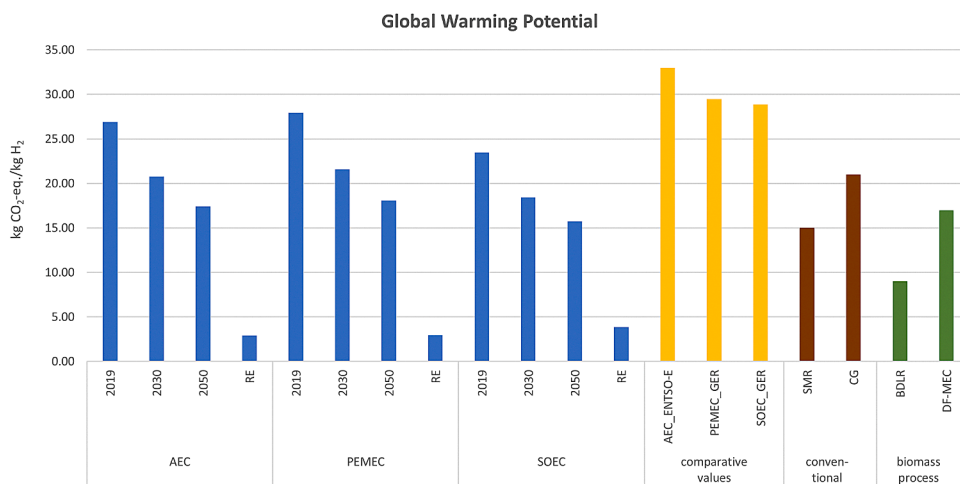


Fig. 8. GWP results and comparative values.

Table 7
PEMEC stack and BoP components.

PEMEC: Stack and BoP components [5,29,43, *]			
	BoP components		
1	Power electronics (rectifier, voltage adaption)	14	Buffer tank
2	Control panel/electronics	15	Container
3	Tubing and pump	16	Foundation (concrete)
4	Gas purification (de-oxo) & water treatment		Stack components
5	Water-gas separator	17	End plate
6	Valve	18	Bipolar plate
7	Back pressure regulator	19	Membrane polymers
8	Ion exchanger	20	Electrocatalyst anode
9	Heat exchanger	21	Electrocatalyst cathode
10	Frequency converter diaphragm compressor	22	Current collector
11	Diaphragm, for diaphragm compressor	23	Bolts and screws
12	Container with pipes and fittings for diaphragm compressor	24	Gasket
13	Water purifier & feed tank		* own calculations/assumptions

Comparison of CO₂-eq. results with values in g CO₂/km of conventional fuels

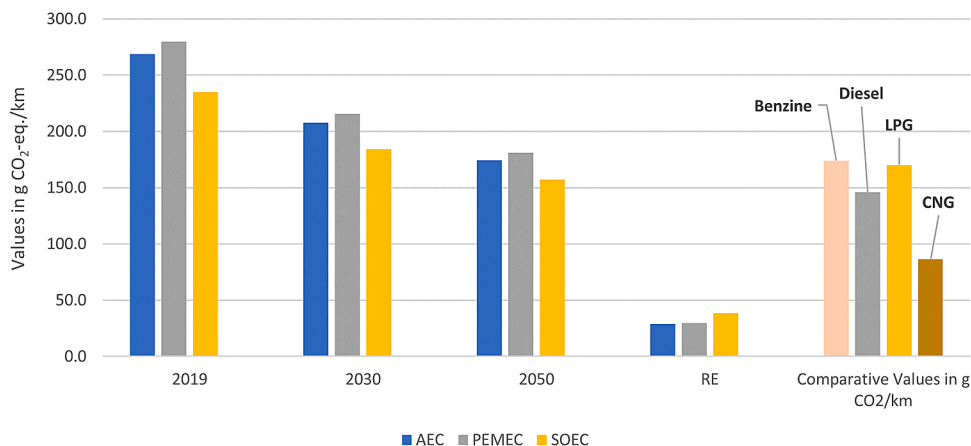


Fig. 9. Comparative values of conventional fuels [70].

3.1.1. Comparison of the GWP results with other LCA studies and hydrogen production processes

As stated above, LCA results from other studies are difficult to compare due to different approaches and assumptions. The comparative values mentioned in Section 1.3 are higher than the CO₂-eq. results of the 1 MW water electrolysis technologies. This can be seen in Fig. 8. The reason is that past energy mixes with a higher share of fossil fuels were considered [5,18], and different assumptions regarding the energy demand of the electrolysis technologies were made [5,25]. Note that the value published by Zhang et al. of around 275 g CO₂-eq./MJ [17] has been converted to approx. 33 kg CO₂-eq./kg H₂ by a factor of 33.33 kWh/kg H₂ according to [66].

For the comparison with conventional processes, the following two processes have been considered. Steam methane reforming (SMR), where hydrogen is produced out of natural gas by the reaction of water with hydrocarbons [5], and coal gasification (CG), where coal is oxidated partially, e.g., by oxygen or steam, into a fuel gas (syngas consisting of hydrogen and carbon monoxide) which can further be processed by the water gas shift reaction in order to produce more hydrogen [67].

In summary, only the values referring to the RE energy scenario are

Table 9 Results in g CO₂-eq./km.

g CO ₂ -eq./km	AEC	PEMEC	SOEC
2019	268.7	279.4	234.8
2030	207.5	215.6	184.3
2050	174.3	181.0	157.2
RE	29.0	29.4	38.4

significantly lower than the values of 15 kg CO₂-eq./kg H₂ (SMR) [17] and 21 kg CO₂-eq./kg H₂ (CG) [17]. While the value of SMR is in the range of 2050's results, the value of CG is in the range of 2030's results (see. Fig. 8).

Regarding the biomass processes, Biomass-Derived Liquid Reforming (BDLR), where biomass products, such as ethanol, are reformed for hydrogen production [68], and Dark Fermentation-Microbial Electrolysis Cell (DF-MEC), where hydrogen is produced from biomass products, such as sugar beet juice, through fermentation [69], have been considered for comparison purposes. As in comparison with the conventional processes, only the RE scenario shows significantly lower results than the biomass processes, which can be seen in Fig. 8. While the value of 9 kg CO₂-eq./kg H₂ (BDLR) [18] is in between 2050's and the RE scenario results, the value of 17 kg CO₂-eq./kg H₂ (DF-MEC) [18] is only in the range of 2050's results.

Overall, the electricity demand of the hydrogen production has the highest impacts on the GWP with a share of more than 90%. Thus, a greener hydrogen production with respect to the CO₂-eq. is only possible if energy mixes consist of no or just little shares of fossil fuels since these are the main drivers of the CO₂-eq. Therefore, an energy mix with a high share of renewables, such as wind and solar energy, enables a greener

Table 10 Comparative values and results of the RE scenario.

Comparative values in g CO ₂ /km and results of the RE scenario in g CO ₂ -eq./km			
Benzine	174.0	AEC*	29.0
Diesel	145.8	PEMEC*	29.4
LPG	170.1	SOEC*	38.4
CNG	86.4		

* values in g CO₂-eq./km

	AEC	PEMEC	SOEC	
Size in kW	4.63	4.82	3.78	kWh/Nm ³ of H ₂
1000	216.0	207.5	264.6	Nm ³ of H ₂ /h
	* 0.0893 kg/Nm ³ under normal condition 1 bar, 15 °C [29]			
1000	19.29	18.53	23.62	kg of H ₂ /h
	* 8000 h/year			
1000	154,298	148,216	188,995	kg H ₂ per year
	* 100 km			
1000	15,429,806	14,821,577	18,899,471	km per year
	: 15.000 km/car (in 1 year)			
1000	1,029	988	1,260	cars per year

Fig. 10. Number of cars driven by hydrogen.

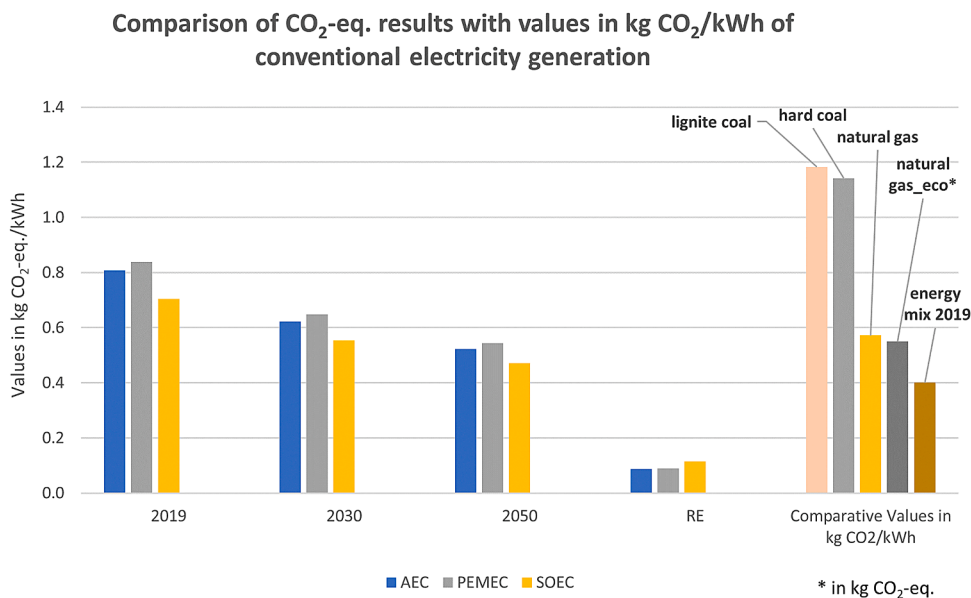


Fig. 11. Comparative values of electricity generation [71,72].

hydrogen production in the future in Germany, presupposed, the expansion of the renewables regarding wind and solar energy is being pushed forward.

3.1.2. Comparison of the GWP results with CO₂ emissions of conventional fuels and electricity generation

In this section, it is assumed that the produced hydrogen is used as a fuel for cars and for electricity generation in order to compare the results with comparative values of conventional alternatives [70–72]. To compare the results in g CO₂-eq./km with comparative values of conventional fuels, the CO₂-eq. results have been divided by 100 km since 1 kg H₂ has a range of 100 km according to reference [8]. Thus, the results shown in Table 9 emerge.

The 2019's and 2030's results are above the comparative values of the conventional fuels in Fig. 9, while the 2050's results are in the range of benzine, diesel, and LPG (Liquefied Petroleum Gas). Therefore, only the RE energy scenario provides results that are significantly below the values of the considered conventional fuels. Thus, green produced hydrogen has the potential to be the climate-friendly oil of tomorrow

and can help to reduce the CO₂ emissions in order to mitigate climate change.

To demonstrate the CO₂ reduction potential of hydrogen as a fuel for cars more clearly, the RE scenario results and the CO₂ emissions of the conventional fuels are shown in Table 10. The values for benzine and LPG (in g CO₂/km) are approx. 6 times higher than the values for hydrogen produced by AEC and PEMEC technology (in g CO₂-eq./km). Regarding diesel and CNG (Compressed Natural Gas), the factor is around 5 times (diesel) and 3 times higher (CNG). On the other hand, the results of the SOEC technology are around 4.5 times (benzine and LPG), 4 times (diesel), and 2 times (CNG) lower in comparison to the conventional fuels. Consequently, as stated above, green produced hydrogen as a fuel for cars has a tremendous potential to help reduce CO₂ emissions, achieve climate goals, and mitigate climate change.

According to the calculation in Fig. 10, approx. 1,029 (AEC), 988 (PEMEC), and 1,260 (SOEC) cars can be driven by hydrogen per year, under the assumption of an annual driving distance of 15,000 km [73] and a driving distance of 100 km per kg H₂ [8]. This calculation gives a rough overview to show how many cars can be driven by the produced

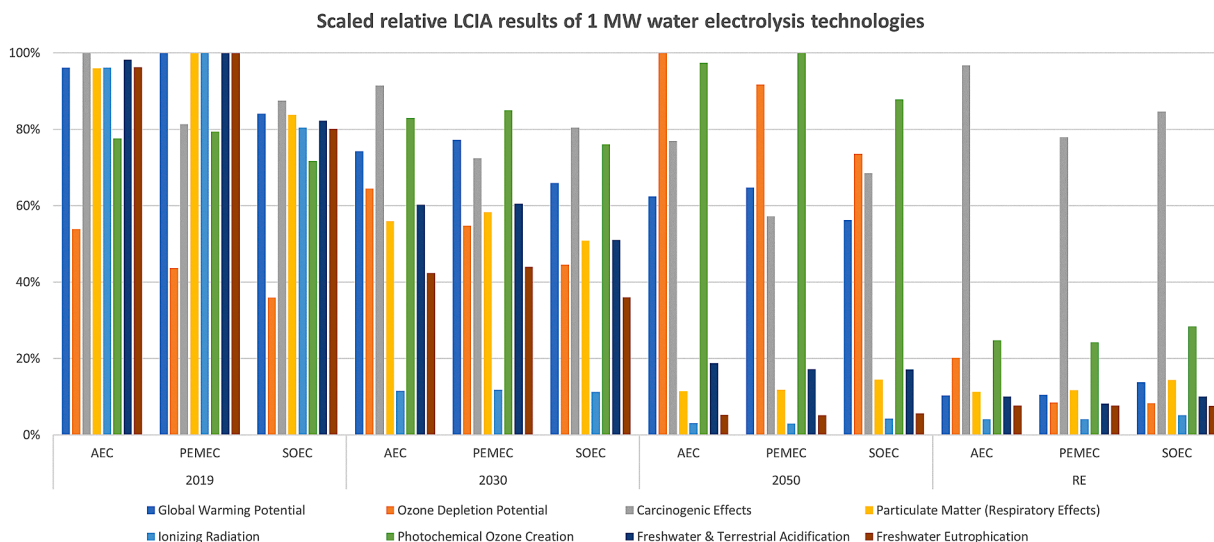


Fig. 12. Scaled relative LCIA results of 1 MW water electrolysis technologies.

Table 11
Results in kg CO₂-eq./kWh.

kg CO ₂ -eq./kWh	AEC	PEMEC	SOEC
2019	0.806	0.838	0.705
2030	0.623	0.647	0.553
2050	0.523	0.543	0.472
RE	0.087	0.088	0.115

hydrogen of the technologies. In addition, the calculation underlines the potential of hydrogen as a climate-friendly oil of tomorrow.

Moreover, to compare the results with comparative values of conventional electricity generation, the results have been divided by 33.33 kWh/kg H₂ [66]; thus, the following values result (Table 11).

The 2019's and 2030's results are considerably below the values of the electricity generation from lignite and hard coal. However, the results are above the values of the electricity generation from natural gas and the energy mix in 2019, except for the result of SOEC_2030. The value is in between the values of the electricity generation from natural gas (Fig. 11). Furthermore, the 2050's results are in between the values of natural gas_eco and the energy mix in 2019, while only the RE scenario shows results that are substantially lower than the comparative values of the conventional electricity generation. Hence, only hydrogen produced by the RE energy scenario provides a potentially more environmentally friendly option regarding the considered conventional alternatives. Thus, green produced hydrogen has the potential to replace fossil fuels for electricity generation in order to help reduce CO₂ emissions and mitigate climate change.

Note that the CO₂ emissions of the conventional alternatives are being compared to potential CO₂-eq. including other substances, such as methane. While the CO₂ emissions in kg CO₂/kWh, derived from [71, 72], barely differ from the Umberto+ results in kg CO₂-eq./kWh, the values in g CO₂/km based on [70] and the corresponding values in g CO₂-eq./km from Umberto+ deviate significantly [SI Table 7-8]. This is because car production processes and maintenance of infrastructure were considered by ecoinvent to depict the processes. Thus, the CO₂

emissions of the conventional alternatives, and not the CO₂-eq. results by the Umberto+ software, have been chosen for classification purposes. Because of that, the potential environmental impacts of other processes, such as car production processes or the maintenance of infrastructure, are not included in the results. Consequently, the comparison is more realistic, even if the CO₂ emissions and CO₂-eq. can only be compared to a limited extent for the above-mentioned reason.

Moreover, the fuel cell process that converts hydrogen into electricity has only a slight impact on the results. Hence, the process has not been considered in the study. For example, the result of the 1 MW_AEC_2019 scenario including the fuel cell process is approx. 26.88 kg CO₂-eq. Without considering the fuel cell process, the result is approx. 26.87 kg CO₂-eq. Therefore, the impact is insignificant. To model the fuel cell process, the ecoinvent processes "fuel cell production, polymer electrolyte membrane, 2 kW electrical, future [RoW]" as well as "maintenance, polymer electrolyte membrane fuel cell 2 kW electrical [RoW]" [21] have been chosen due to limited options. Moreover, for the conversion process of hydrogen into electricity, no electricity has been considered. Therefore, the results increase if electricity from the grid is considered, unless the electricity demand is covered through the own use of the produced electricity.

3.2. LCIA results

In this section, the LCIA indicators are described, and the main reasons for the change in the results are discussed, without considering the GWP which has been analysed in detail above. However, the GWP results are shown in Fig. 12, and have been considered for comparison purposes. Moreover, the maximum values of the LCIA indicators, which have been used to scale the relative LCIA results in Fig. 12, are presented in Table 12. Subsequently, a comparison of the results is carried out in 3.2.3 to show the potentially most environmentally friendly technology for each energy scenario. The percentage deviations of the results for the comparison can be found in the SI Tables 10-12.

Table 12
Maximum results of LCIA indicators.

Technology	Energy scenario	Abbreviation	Main drivers	Value	Unit per kg H ₂
PEMEC	2019	GWP	Electricity production lignite coal	2.79E+01	kg CO ₂ -eq.
AEC	2050	ODP	Tetrafluoroethylene production	3.68E-06	kg CFC-11 eq.
AEC	2019	CE	Chromium steel production	2.28E-07	CTUh
PEMEC	2019	PM	Electricity production biogas burned	1.99E-06	disease incidences
PEMEC	2019	IR	Electricity production nuclear	5.93E+00	kg U ²³⁵ -eq.
PEMEC	2050	POC	Electricity production natural gas	5.19E-02	kg NMVOC-eq.
PEMEC	2019	Acid.	Electricity production biogas burned	3.17E-01	mol H ⁺ -eq.
PEMEC	2019	Eutr.	Electricity production lignite coal	3.82E-02	kg P-eq.

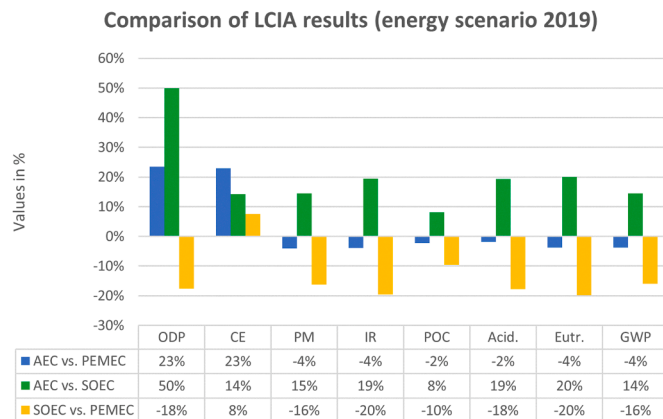


Fig. 13. Comparison of the LCIA results applying the energy scenario of 2019.

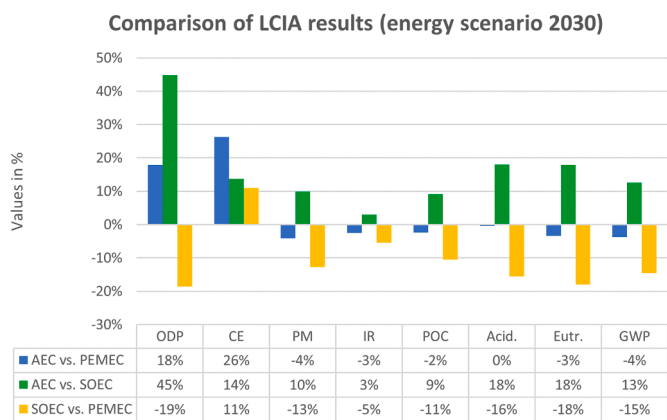


Fig. 14. Comparison of the LCIA results applying the energy scenario of 2030.

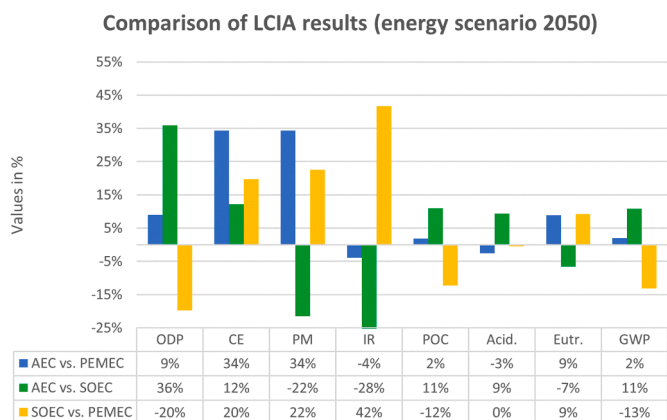


Fig. 15. Comparison of the LCIA results applying the energy scenario of 2050.

3.2.1. Maximum values of the LCIA indicators

The maximum values of the LCIA indicators are listed in Table 12. These values have been used to scale the relative LCIA results shown in Fig. 12. The 1 MW PEMEC technology using the energy scenario in 2019 shows the maximum values for the GWP, particulate matter, ionizing radiation, freshwater & terrestrial acidification, and freshwater eutrophication indicators, while the highest value for photochemical ozone creation refers to 1 MW PEMEC using the energy scenario in 2050. Furthermore, the maximum values for the carcinogenic effects and ODP refer to the 1 MW AEC technology utilizing the 2019's and 2050's energy scenarios, respectively.

The maximum values of the indicators linked to the PEMEC technology are mainly caused by the (higher) energy demand for the hydrogen generation. This also applies to the maximum values of the AEC technology, even though the chromium steel production process (regarding CE) and the tetrafluoroethylene production process (regarding ODP) have a significant impact on the results as well.

3.2.2. Description of the LCIA indicators and discussion of the main reasons for the change in the results

The ozone depletion potential (ODP) indicator, which expresses potential negative effects on the stratospheric ozone layer [32], increases from 2019 to 2050 by more than 35% across all electrolysis systems (see Fig. 12). The main driver for this rise is the electricity production from natural gas since the share of natural gas in the energy mix in 2050 has almost doubled (see Fig. 3). The sharp drop of the ODP in the RE scenario occurs because natural gas is not included in the energy mix anymore. The ozone depletion leads to more UVB (Ultraviolet B) radiation due to less protection from sun rays. This can lead to

effects on human health as well as affect the growth process of plants [74].

The next indicator, carcinogenic effects, indicates the potential estimated rise of disease cases per kg of a substance emitted. The unit of the indicator is the comparative toxic unit for humans (CTUh) [32]. The indicator decreases from 2019 to 2050 by more than 18% and rises again by more than 15% when applying the RE scenario. The main reason for the decrease is the decline of lignite coal in the energy mix to zero percent, whereas the increase of wind energy (onshore) is the main cause for the rise.

Furthermore, the indicator respiratory effects, also known as particulate matter, describes the potential effects on human health through fine dust emissions and is measured in disease incidences/kg PM2.5 [33]. The indicator declines sharply from 2019's scenario to the RE scenario by more than 65% across all electrolysis systems. The main reason is the decline of produced electricity from biomass, which is the main driver of the respiratory effects. Concerning the health effects, particles smaller than 10 µm cause the main problems to human health, especially heart and lung diseases [75].

In addition, the ionizing radiation indicator, that calculates potential impacts on human health caused by radionuclides emissions [32], declines by more than 65% from 2019's to 2030's energy scenario. The nuclear power plants, which are the main driver of the indicator, are no longer running due to the nuclear phase-out; thus, the results sink sharply. Ionizing radiation can affect the DNA through mutation and cause different types of cancer [32].

Moreover, the results of photochemical ozone creation increase slightly from the energy scenario in 2019 to 2050 because of the natural gas share increase in the energy mix. Subsequently, the indicator decreases by more than 55% with respect to the RE scenario since natural gas as the main driver of 2050's results is not included in the energy mix anymore. Photochemical ozone can cause near to ground produced tropospheric ozone, also known as summer smog [32]. Moreover, summer smog can affect human health through heart and lung complications [76].

Further, the freshwater & terrestrial acidification indicator, which describes the acidification potential of soil and freshwater [33], declines constantly primarily due to the decline of produced electricity from biomass in the energy mixes. Moreover, the absence of natural gas in the RE scenario is also a main reason for the decline of the indicator.

The last indicator, freshwater eutrophication, measures the potential impacts on rivers and lakes by a surplus of nutrients. The indicator takes only phosphorus emissions into account [32] and drops sharply from 2019 to 2050 by more than 70%. The reason is primarily the decline of hard and lignite coal to zero percent in the energy mix.

Besides that, the additional manufacturing energy has little impact on the LCIA results (see Table 5 in the SI). Hence, no further analysis of the additional manufacturing energy is carried out.

3.2.3. Comparison of the LCIA results

The comparison of the 1 MW water electrolysis technologies is shown in Figs. 13–16. Moreover, the results are attached in the SI (Section 5, Table 9), where the maximum and minimum values of each single LCIA indicator are marked in red and green, respectively. The interpretation of the results is explained in the following using Fig. 13.

The AEC result of the LCIA indicator ODP is 23% higher compared to PEMEC. Hence, AEC has a greater potential environmental impact concerning the ODP than PEMEC. A negative value leads to the opposite interpretation. For example, the potential environmental impact of AEC regarding particulate matter (PM) is 4% lower compared to PEMEC, meaning that AEC is preferable to PEMEC with respect to the LCIA indicator. This evaluation process has been carried out constantly for each indicator to identify the potentially most environmentally friendly technology for each energy scenario, as shown in the following discussion.

With regard to the energy scenarios in 2019 and 2030, the 1 MW

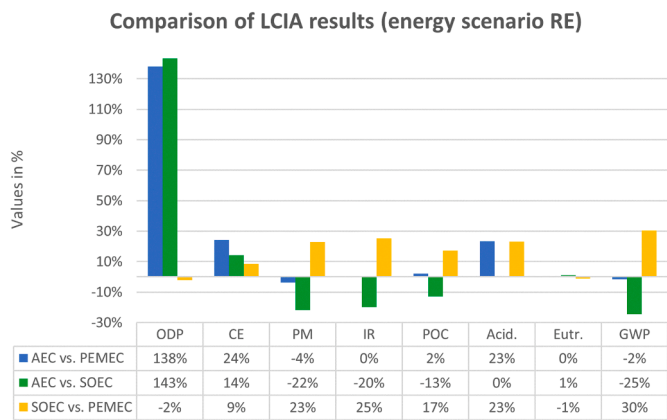


Fig. 16. Comparison of the LCIA results applying the RE energy scenario.

SOEC technology shows lower results in comparison to the AEC technology for all indicators considered (see Figs. 13 and 14). The same applies to SOEC in comparison to PEMEC, except for the carcinogenic effects. Hence, SOEC can be designated as potentially the most environmentally friendly technology for the energy scenarios in 2019 and 2030, mainly due to the lower energy demand. When comparing the results of the potential environmental impacts of AEC and PEMEC for the energy scenarios in 2019 and 2030, PEMEC can be stated as more potentially environmentally friendly than AEC, even though PEMEC shows the highest values for 6 out of 8 LCIA indicators. However, these values only differ slightly, while the difference of the other 2 indicators —ODP and carcinogenic effects— is significant (see Figs. 13 and 14). Besides this, PEMEC can be classified as potentially the most environmentally friendly technology for the energy scenario in 2050 and the RE scenario, considering all 8 LCIA indicators, since the technology shows lower results in comparison to SOEC, especially regarding the indicators of carcinogenic effects, ionizing radiation, and particulate matter. The reasons for the higher results of these indicators are, on the one hand, mainly due to the assumed external heat supply for the hydrogen production by SOEC, modelled with the process "heat, district or industrial, other than natural gas" in Umberto+. On the other hand, the change in the energy mix with a higher proportion of wind and solar energy leads to a lower impact of the energy demand of the water electrolysis technologies on the results. For these reasons, SOEC is not the potentially most environmentally friendly technology for the scenario in 2050 and the RE scenario.

Furthermore, AEC can be classified as more potentially environmentally unfriendly than PEMEC regarding the energy scenario in 2050 and the RE scenario, in particular, because of higher results for ODP, carcinogenic effects, and freshwater & terrestrial acidification (see Figs. 15 and 16). The higher results emerge, on the one hand, due to the gasket production (ODP) and, on the other hand, because of the higher steel (carcinogenic effects) and nickel (freshwater & terrestrial acidification) requirement. Therefore, AEC is potentially the most environmentally unfriendly technology concerning the energy scenario in 2050 and the RE scenario. This also comprises the comparison with the SOEC technology, mostly due to the higher ODP values. Without including the ODP indicator in the evaluation, SOEC can be stated as potentially the

Table 13 Ranking of the technologies.

Energy scenario	1	2	3
2019	SOEC	PEMEC	AEC
2030	SOEC	PEMEC	AEC
2050	PEMEC	SOEC	AEC
RE	PEMEC	SOEC	AEC

most environmentally unfriendly technology when applying the energy scenario in 2050 and the RE scenario. Table 13 shows the ranking of the water electrolysis technologies for each energy scenario considering all LCIA indicators under study.

4. Conclusion

In this study, potential environmental impacts –in particular the CO₂-eq.– of a greener hydrogen production have been analysed considering the three major technologies AEC, PEMEC, and SOEC. For this, different energy scenarios with an increasing share of wind and solar energy for a greener hydrogen production have been selected. The aims of the study were, on the one hand, to analyse how the CO₂-eq. change when applying the different energy scenarios, which technology accounts for the lowest CO₂-eq. for each scenario, and which technology is potentially the most environmentally friendly one for the respective energy scenario taking all analysed indicators into account. On the other hand, the aim was to compare the results of the CO₂-eq. with conventional and other hydrogen generation processes, CO₂ emissions of conventional fuels for cars, and conventional electricity generation, assuming that the produced hydrogen is used as a fuel for cars or to generate electricity. The study concludes that the CO₂-eq. decrease with an increasing share of wind and solar energy in the energy mix, with SOEC showing the lowest CO₂-eq. for the energy scenarios in 2019, 2030, and 2050. This applies to AEC for the RE scenario. Furthermore, SOEC is potentially the most environmentally friendly technology for the energy scenarios in 2019 and 2030, taking all analysed indicators into account. This applies to the PEMEC technology for the energy scenario in 2050 and the RE scenario. In this respect, from the perspective of the environment and without considering the cost side, the production of hydrogen is recommended with the SOEC technology for the energy scenarios in 2019 and 2030 to keep the potential environmental impacts as low as possible, while this applies to the PEMEC technology for the energy scenario in 2050 and the RE scenario. Regarding the comparative values, only the RE energy scenario with wind and solar energy shows significantly lower results. Consequently, green produced hydrogen can help to reduce CO₂ emissions and minimize environmental impacts, thus being a sustainable alternative compared to conventional options. For this, the expansion of wind and solar energy in Germany is essential, as the share of these energies in the energy mix in 2019 was only around 33%. In addition, the expansion of wind and solar energy to produce green hydrogen in Germany would support the government's goal of becoming a world leader in the field of hydrogen by 2030. Besides this, green produced hydrogen can help to achieve the goals of the European Union and Germany with regard to the decarbonization of industry, transport, electricity generation, and buildings. Overall, green produced hydrogen can help to reduce CO₂ emissions significantly and mitigate global warming, which is one of the greatest challenges of our time and we face across borders. However, the expansion of wind and solar energy needs to be accelerated considerably for this. Then green produced hydrogen has the potential to be the climate-friendly mineral oil of tomorrow and can, therefore, help mitigate climate change.

5. Limitations

In this section, the limitations of the study are addressed. The ecoinvent database is limited in terms of the choice of material and recycling processes. Therefore, the materials LSM and iridium have been self-created using literature. The self-created processes include fewer potential environmental impacts compared to standard ecoinvent processes due to a lack of information in the literature. Nevertheless, the impacts on the results are neglectable since the shares of these materials on the mass balance are little. Concerning the disposal phase, hardly any recycling processes were available in the database. With a wider range of recycling processes in the database, the potential environmental impacts

would have been lower since recycling processes of materials (e.g., copper, aluminium) can cause fewer emissions than a newly produced material, including the whole manufacturing process starting with the raw material extraction. However, the disposal phase has just a minor impact on the overall results. Hence, the impact on the result is negligible. Since the SOEC technology is not yet commercially available and still is in the developing stage, hardly any data regarding the stack and BoP were available. This can be seen as a limitation. Nonetheless, the fundamental data collection for the research study offers a comprehensive opportunity for further research projects.

CRedit author statement

Niklas Gerloff: Term, Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing-Original Draft, Revision-Editing, Visualization, Supervision, Project administration.

Note

The results can be projected to other countries and circumstances, even though the work was done taking only the (forecasted) energy scenarios of Germany into account. Therefore, this work is useful for decision makers and researchers around the world working in the field of sustainability of energy conversion and storage technologies.

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Declaration of Competing Interest

The author declares that he has no known competing financial interests or personal relationships that could have influenced the work of this research article.

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Supplementary materials

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Publikation 2

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Abstract: Germany's energy system is transitioning to a more renewable one, leading to new challenges, such as in the wintertime, when solar and wind energy are less accessible. Power to methane (PtM) can, thusly, serve as a long-term storage solution, as the natural gas grid already exists, therefore reducing costs. The study aims for analysis of potential environmental impacts of synthetic natural gas (SNG) production in different PtM plants—including the electrolysis technologies such as alkaline electrolysis (AEL), polymer electrolysis membrane (PEM), and solid oxide electrolysis cell (SOEC)—applying various energy scenarios—2019, 2030, 2050, and renewable energy (RE)—to show which technology accounts for the lowest CO₂ equiv and is potentially the most environmentally friendly, and to compare results to the potential environmental impacts of conventional natural gas production and CO₂ emissions of conventional alternatives. The PtM-SOEC shows the lowest CO₂ equiv for the scenarios in 2019, 2030, and 2050—PtM-AEL for RE—and is potentially the most environmentally friendly technology regarding 2019's and 2030's scenarios. This applies to PtM-PEM for 2050's scenario as well as RE's. The conventional natural gas production accounts for less potential environmental impacts than SNG. Only the RE scenario results are lower or within the range of CO₂ emissions of considered conventional alternatives.

Comparative Life-Cycle Assessment Analysis of Power-to-Methane Plants Including Different Water Electrolysis Technologies and CO₂ Sources While Applying Various Energy Scenarios

Niklas Gerloff*

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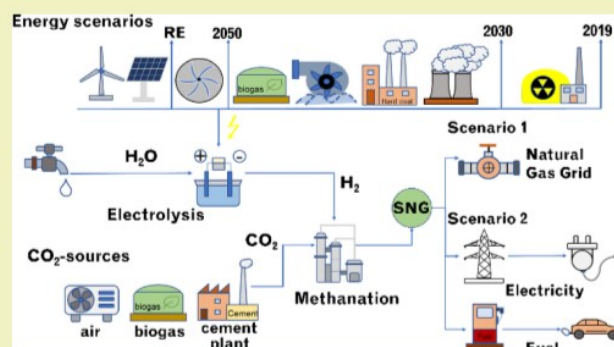
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ABSTRACT: Germany's energy system is transitioning to a more renewable one, leading to new challenges, such as in the wintertime, when solar and wind energy are less accessible. Power to methane (PtM) can, thusly, serve as a long-term storage solution, as the natural gas grid already exists, therefore reducing costs. The study aims for analysis of potential environmental impacts of synthetic natural gas (SNG) production in different PtM plants—including the electrolysis technologies such as alkaline electrolysis (AEL), polymer electrolysis membrane (PEM), and solid oxide electrolysis cell (SOEC)—applying various energy scenarios—2019, 2030, 2050, and renewable energy (RE)—to show which technology accounts for the lowest CO₂ equiv and is potentially the most environmentally friendly, and to compare results to the potential environmental impacts of conventional natural gas production and CO₂ emissions of conventional alternatives. The PtM-SOEC shows the lowest CO₂ equiv for the scenarios in 2019, 2030, and 2050—PtM-AEL for RE—and is potentially the most environmentally friendly technology regarding 2019's and 2030's scenarios. This applies to PtM-PEM for 2050's scenario as well as RE's. The conventional natural gas production accounts for less potential environmental impacts than SNG. Only the RE scenario results are lower or within the range of CO₂ emissions of considered conventional alternatives.

KEYWORDS: power to methane, synthetic natural gas, CO₂ source, life-cycle assessment, environmental impacts, greener production



INTRODUCTION

Due to the enhanced climate change, the Paris agreement was arranged to limit global warming to lower than 2 °C in comparison to the preindustrial time period.¹ The target of the federal government of Germany is in line with the Paris agreement and aims to reduce CO₂ emissions by 88% by 2040 in comparison to the base year 1990.² Hence, an expansion of wind and solar energy plants is a substantial part of the German energy system transition with an estimated increase of the installed capacity of around 83 GW until 2030 in comparison to the year 2020 based on a scenario drafted by Agora Energiewende.³ This equals an increase of more than two-thirds. However, new challenges can arise regarding the energy system transition. For example, what will happen throughout the wintertime when hardly any wind and solar energy is accessible for electricity generation? How are the fluctuations balanced? Hence, an estimated amount of 35 TWh is required as a reserve to cover the electricity supply and demand in Germany as well as to avoid a blackout.^{4,5} Some short-term storage technologies that provide energy in the range of minutes or hours are not sufficient for this time period because of their limited capacity.⁶ Thus, only compressed air storage, pumped hydro, or power-to-gas (PtG) technologies with an adequate storage capacity are suitable as a

long-term storage solution to meet the electricity supply and demand during the wintertime.^{7,8} However, only PtG is appropriate as a promising long-term storage technology since compressed air storage and pumped hydro are not suitable because of geological, topographical, and economic conditions.⁷ Moreover, the main advantage for PtG as a long-term storage solution is the already existing natural gas (NG) grid infrastructure in Germany with a length of approx. 500,000 km and a storage capacity of around 350 TWh.⁵

Power to Gas. What is PtG? PtG means the conversion of electricity into gas, mainly the conversion of electricity into hydrogen by water electrolysis (power to hydrogen) that can be fed into the NG grid (permitted volumetric percentage for H₂ in the range of 1% to max. 10%).^{9,10} The produced hydrogen can further react with carbon dioxide to make synthetic natural gas

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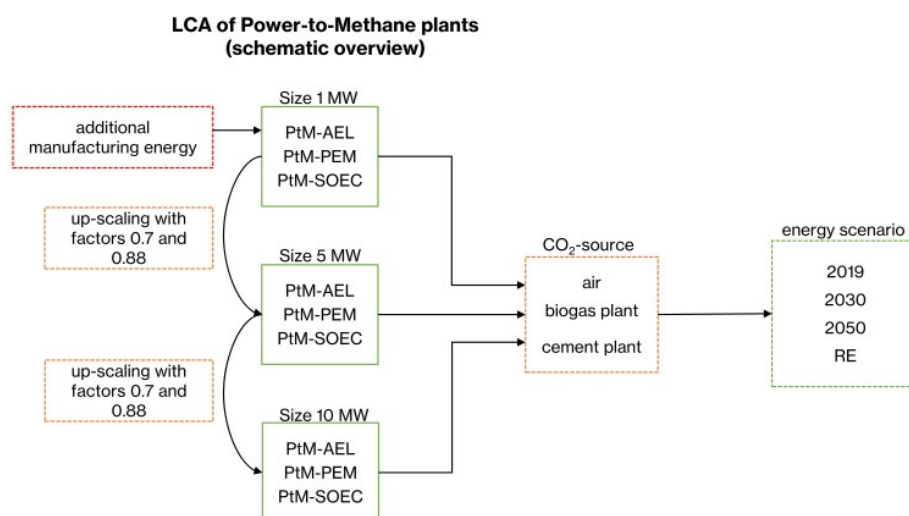


Figure 1. Schematic overview of the LCA study.

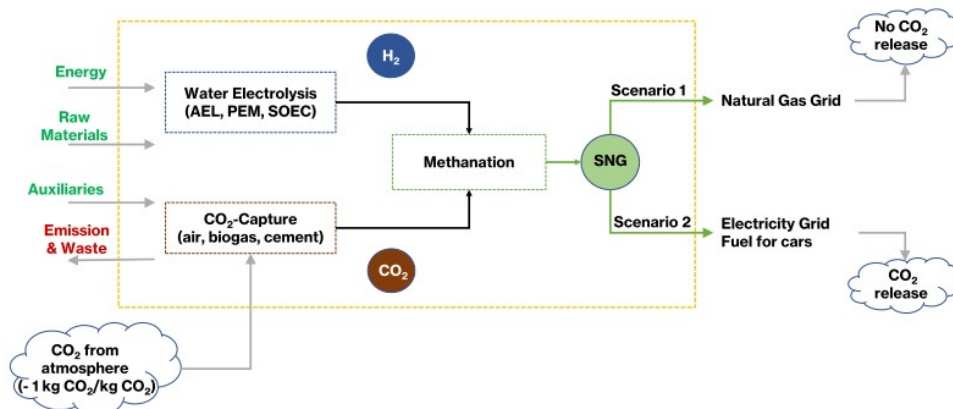


Figure 2. System boundary of the PtM process.

(SNG), its main component being CH_4 (methane). Thus, the produced SNG can be fed into the NG grid as well after dehydration and conditioning since the characteristics of SNG and NG hardly differ.^{11,12}

In summary, the target of the federal government of Germany—along with the Paris agreement—leads to an expansion of wind and solar energy plants that may lead to uncertain electricity supply during the wintertime. A solution for this problem is power to methane (PtM), where the produced SNG can be fed in the already existing NG grid for further utilization (electricity generation). Also, the expansion of wind and solar energy plants enables a greener SNG production that can help to reach the government's goal and mitigate climate change. Moreover, the focus on topics such as climate change and sustainability in the German society (Fridays for Future)¹³ are beneficial for this work, in which the life-cycle assessment (LCA) and the associated potential environmental impacts of various PtM plants are analyzed.

Previous Studies on PtG and Goals of This Study. There are previous studies in the field of PtG.^{14–23} Most of the previous studies are based on the concept of power to hydrogen, whereas only a few address the concept of PtM.^{11,24,25} Moreover, previous studies are mainly focused on techno-economic aspects and barely take environmental aspects into

account.¹¹ When considering environmental aspects, the global warming potential (GWP) is the most significant. Other indicators, such as ozone depletion, carcinogenic effects, or ionizing radiation, are less considered.^{11,25,26} Besides these, there is no study to the knowledge of the author available that carried out a comprehensive LCA on PtM plants considering different water electrolysis technologies, CO_2 sources—air, biogas, and cement plant—and energy scenarios—2019, 2030, 2050, and renewable energy (RE) (including only wind and solar energy)—with an increasing share of wind and solar energy for a greener SNG production to show which technology is potentially the most environmentally friendly one for the respective scenario as well as to compare the results with potential environmental impacts of conventional NG production. Moreover, novelty can also be found in the comparison of greener-produced SNG with conventional alternatives in order to show a reduction potential of CO_2 emissions, assuming that the SNG is used for electricity generation and as a fuel for cars. A reason why hardly any LCA studies on PtM plants have been done to date is mainly due to the limitation of data availability, in particular, regarding polymer electrolysis membrane (PEM) Balance-of-Plant (BoP)^{11,27} and solid oxide electrolysis cell (SOEC) stack and BoP^{28,29} components. Therefore, the study aims to fill the research gaps concerning the LCA of PtM plants.

For this, two scenarios have been created (see Figure 2). The first scenario considers only the SNG production for the direct storage into the NG grid and takes an environmental credit of $-1 \text{ kg CO}_2/\text{kg CO}_2$ for the captured CO_2 into account because the CO_2 is withdrawn from the atmosphere and not released again through combustion processes (scenario 1, Figure 2). Therefore, the produced SNG for storage purposes can be seen as a cache for CO_2 . Subsequently, the results are compared with each other to show which technology is potentially the most environmentally friendly one. Further, they are compared with the potential environmental impacts of conventional NG production. On the other hand, the produced SNG is considered for electricity generation and as a fuel for cars without taking the environmental credit of $-1 \text{ kg CO}_2/\text{kg CO}_2$ into account since the bonded CO_2 is released to the atmosphere during the conversion processes (scenario 2, Figure 2). The results are compared with the CO_2 emissions of conventional electricity generation and conventional fuels for cars. In total, the following research questions will be answered.

1. Which PtM technology shows the lowest CO_2 equiv?
2. Which PtM technology is potentially the most environmentally friendly one regarding the energy scenarios including all analyzed life-cycle impact assessment (LCIA) indicators?
3. How do the LCIA results differ in comparison to the conventional NG production?
4. If the produced SNG is used for electricity generation or as a fuel for cars, how do the results differ in comparison to the CO_2 emissions of conventional alternatives?

Additionally, the manufacturing energy of stack and other components has been estimated as there are hardly any given values in the ecoinvent database version 3.5³⁰ and in previous studies related to this topic,^{11,17,18,20–23} except for PEM and SOEC stacks.^{31,32} Different energy scenarios have been applied in this LCA study to analyze the SNG production from a greener perspective. Moreover, energy is the most sensitive parameter as well as the main driver for the potential environmental impacts, so this parameter has been treated with more care.¹¹ Consequently, the energy mix in 2019, future scenarios for 2030 and 2050, as well as an energy mix that only consists of wind and solar energy have been considered (see Figure 3).^{27,33,34} Also, more environmental impacts than the GWP will be addressed in this work (see Table 2).

METHODOLOGY

The methodology comprises the sections “LCA Study Scope” and “PtM technologies and the generation of the life-cycle inventory (LCI) data”. While the LCA study scope is illustrated in the following paragraph, the other section is discussed in Supporting Information Section 1.

LCA Study Scope. The LCA study scope includes the schematic overview and general information, the system boundary, the PtM plant and stack lifetimes, the functional unit, the scaling factors, and the additional manufacturing energy. Furthermore, the energy scenarios, the estimation of the produced amount of SNG, the operating data as well as the selected disposal processes of the materials, and the chosen LCIA indicators are described.

Schematic Overview and General Information. Figure 1 shows the schematic overview of the LCA study.

To summarize the scheme in brief, the LCI data of the PtM plants have been generated based on 1 MW alkaline electrolysis

(AEL), PEM, and SOEC systems. Further, the LCI data of the other plant sections (methanation, direct air capture (DAC), biogas plants, and CO_2 capture from cement plants) have been added. The data are based on the literature, manufacturer information, expert opinions, and own calculations, as well as background data from the ecoinvent database version 3.5. Subsequently, the values have been scaled up (see section scaling factors) to 5 and 10 MW. The results of the potential environmental impacts have been created with the Umberto LCA+ software version 10.0.3.³⁵ In total, 108 LCA models have been modeled by taking the four different energy scenarios into account.

As recommended by ISO 14040 and 14044, the LCA study avoids complex allocation.^{11,36,37} For this reason, the allocation cut-off method has been chosen since it is assumed that the emerging oxygen during the hydrogen production process is released into the atmosphere. Thus, the PtM process is considered as a single output process to avoid complex allocation.³⁸ Hence, the method for multioutput processes—allocation at point of substitution (APOS)—cannot be applied in this study as well as the method for long-term future scenarios—consequential method—due to higher uncertainties.³⁹

The ecoinvent processes of Europe (RER and Europe without Switzerland) have been selected with respect to the geographical reference. If the option Europe was not available, RoW (rest of the world), GLO (global), or CH (Switzerland) have been chosen. Due to the proximity to Germany, CH is preferred over RoW and GLO. If possible, Germany (DE) has been selected.

For the transportation of the components, two transport ways, each 250 km, have been assumed. While the first transport way relates to the delivery of single items for the manufacturing process, the second transport way relates to the delivery of the components to the location of the PtM plant. The values have been entered in the software in metric ton^*km per kg SNG. To model the transport way, the ecoinvent process transportation with freight lorry >32 metric ton, Euro 6 (RER), has been chosen.³⁰

System Boundary. On the one hand, the system boundary comprises the SNG production for feeding into the NG grid (scenario 1, Figure 2). On the other hand, the system boundary comprises the SNG production and the usage of the SNG for electricity generation and as a fuel for cars (scenario 2, Figure 2). Therefore, as mentioned above, the environmental credit is only considered for the first scenario. Moreover, all processes in relation to energy, raw materials, and auxiliaries have been selected from the ecoinvent database version 3.5.³⁰

PtM Plant and Stack Lifetimes. Regarding the PtM components, a lifetime of 20 years (operating 8000 h/year) has been assumed, except for the stack components. For them, three exchanges have been assumed within 20 years based on data derived from the IndWEDe study that predicts a lifetime of 50,000 h or more for the stacks (2030's scenario).^{40,41}

Functional Unit. The FU has to fulfill two requirements according to ISO 14040. It has to be both scalable and satisfy a function.^{36,38} The function of the SNG is not limited to just one in this study. Therefore, the storage in the NG grid for the wintertime as well as the usage to generate electricity and as a fuel to drive cars are considered as functions of the SNG.¹¹ A reference flow of 1 kg of SNG has been chosen to make the FU scalable. In order to break the weights of the components down to the FU of 1 kg of SNG, the weights have been divided by the assumed, produced amount of SNG in 20 years (see Figure S27

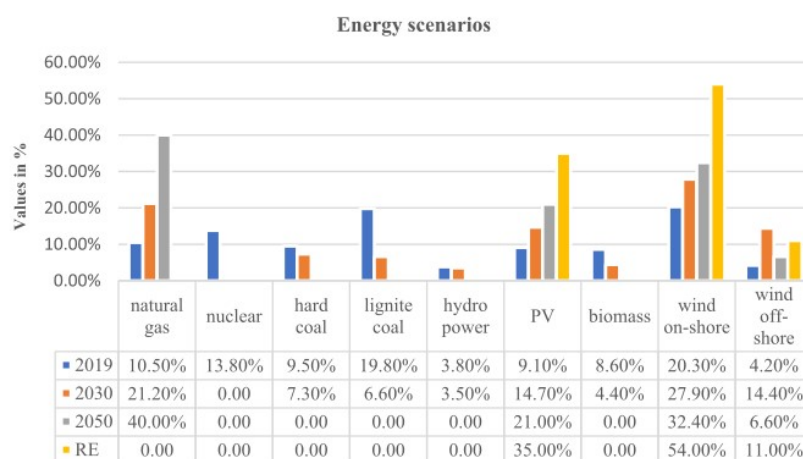


Figure 3. Energy scenarios.

Table 1. Operating Data

operating data per kg SNG	AEL	PEM	SOEC	methanation	DAC	biogas	cement
water demand for H ₂ production (kg/kgSNG) ¹	4.5	4.5	4.5			^a see note below	
heat demand (kWh/kgSNG) ^{2–4}		0.14	2.62		4		4
electricity demand (kWh/kgSNG) ^{5–8}	25.9	27	21.2	0.44	1.03		0.466
KOH kg/kgSNG ⁹	0.0018						
NaOH kg/kgSNG ¹⁰							0.24
MEA kg/kgSNG ¹¹							0.0097
market for chemicals, organics kg/kgSNG ¹²					0.0096		
cooling water (l/kgSNG) ^{13–15}	4.6	4.6	125	6.9	0	15.1	294.5
cooling water for compressors (l/kgSNG) ¹³	40	40	200	air cooling	air cooling	air cooling	air cooling

^as. database value biogas production from grass CH (assumed, that all auxiliaries are included)

in the Supporting Information). Moreover, the stack components have been multiplied with a factor of 3 (see above).

Scaling Factors. As mentioned above, the design of PtM plant components is based on the size of 1 MW AEL, PEM, and SOEC systems. Subsequently, all components have been scaled to 5 and 10 MW PtM systems (applying eq 1) with a scaling factor of 0.88 for stack components and 0.7 for BoP and all other components.^{42,43} The scaling method applied in this study is based on Remer and Chai.⁴⁴ The method has been modified according to Zhang et al., as shown in eq 1.⁴³

$$\frac{C_2}{C_1} = \left(\frac{X_2}{X_1} \right)^b \quad (1)$$

C₁—component 1 (known weight), C₂—component 2 (unknown weight), X₁—capacity of plant or component 1 (e.g., volume or mass flow), X₂—capacity of the plant or component 2 (e.g., volume or mass flow), and b—scaling factor.

The reason for the modification was the lack of information regarding the weight of components. Consequently, the weight of the same component that is used for different volume or mass flows could be estimated because the weight has been scaled up or down according to the volume or mass flows.^{43,45}

Additional Manufacturing Energy. Additional manufacturing energy for components has been estimated since this energy is barely considered in the ecoinvent processes. As an example, the manufacturing process of a heat exchanger is described shortly. To model the manufacturing process, the ecoinvent processes chromium steel production and sheet

rolling chromium steel have been selected.⁴⁶ However, manufacturing steps, such as welding or assembling, are not accounted for in the ecoinvent database; hence, additional manufacturing energy has been added in accordance with the literature. This has been applied for various components (see Section 2 in Supporting Information).

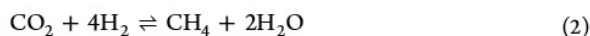
Energy Scenarios. Different energy scenarios for Germany with an increasing share of wind and solar energy have been considered for the purpose of a greener SNG production. Figure 3 shows the composition of the different energy scenarios. The values are derived from refs 27 33, and 34.

The values of the wind energy derived from the literature were not separated in on- and offshore parts. Therefore, this has been done to draw a more realistic picture. For this, the value of 106 TWh (2017)—88 TWh were produced by on- and 18 TWh by offshore windmills—has been considered to split the wind energy in on- and offshore parts.³⁴ Consequently, the onshore windmills produced 83% (88 TWh divided by 106 TWh) of the total wind energy, while the offshore windmills produced 17% (18 TWh divided by 106 TWh). These values have been used to split the total wind energy into on- and offshore parts for each energy scenario, assuming that the values will remain consistent in the future.

The additional manufacturing energy (see Supporting Information Section 2) and the operating energy (see Table 1) have been multiplied with the percentages of the energy types (see Figure 3) in order to split them.

Produced Amount of SNG. The production of SNG in the PtM plants takes place according to the following reaction

equation (see eq 2) since it is assumed that SNG and methane have the same characteristics.^{11,47}



Considering the equation above and assuming 100% yield, approx. 2.74 kg of CO₂ and around 0.5 kg of H₂ are needed to produce 1 kg of SNG based on own calculations following Zhang et al. and the periodic table.⁴⁶ The estimation of the produced amount of SNG during the assumed lifetime of 20 years can be found in Supporting Information Section 3.

Operating Data. As mentioned above, 0.5 kg of H₂ is required to produce 1 kg of SNG. Hence, 25.9 kWh (AEL), 27 kWh (PEM), and 21.2 kWh (SOEC) are needed to produce 0.5 kg of hydrogen according to the corresponding technology.⁴¹ These values are approx. half the values that are required to produce 1 kg of H₂ according to Bareiß et al. and Mehmeti et al.^{27,45} Furthermore, the water demand of 4.5 kg/kg SNG for the hydrogen production (0.5 kg H₂) is based on own calculations according to Zhang et al.⁴⁶ Moreover, it is assumed that the hydrogen produced by AEL and PEM electrolyzers is cooled down by 40 °C from 65 to 25 °C, leading to approx. 4.6 L of cooling water per 0.5 kg of H₂ based on own calculations and assumptions.^{11,48} Table 1 illustrates the operating data for all parts of the PtM process. Further explanations (superscript numbers) of the data can be found in Supporting Information Section 4.

Disposal Processes. The processes shown in Table S22 in Section 5 of Supporting Information have been selected to depict the disposal phase.

LCIA Indicators. Since several methods in Umberto+ are obsolete,⁴⁹ the latest LCIA method in Umberto+, ILCD 2.0 midpoint 2018, has been chosen. However, one exception has been made for the GWP. For this indicator, the IPCC 2013 method has been used. The impact indicators are shown in Table 2. They have been selected with either level I

Table 2. Impact Indicators

nr.	impact indicator	abbreviation	level
1	ozone depletion potential (ozone layer depletion)	ODP	I
2	carcinogenic effects	CE	II
3	particulate matter (respiratory effects)	PM	I
4	ionizing radiation	IR	II
5	photochemical ozone creation	POC	II
6	freshwater and terrestrial acidification	Acid.	II
7	freshwater eutrophication	Eutr.	II
8	global warming potential (GWP 100)	GWP	I

(recommended and satisfactory) or level II (recommended but in need of some improvements), in accordance with the recommendations of the International Life Cycle Data (ILCD) system.⁵⁰

Note that the same LCA methodology has been applied by the author in a previous study regarding the life-cycle assessment of water electrolysis technologies. This study has been accepted for publication. However, it has not been published yet. Hence, the author would like to inform the readership to avoid any kind of self-plagiarism.

RESULTS AND DISCUSSION

The LCIA results of the study that can be found in Figure S28–S30 in the Supporting Information are discussed in this section. Moreover, the research questions stated in the Introduction will

be answered. Since GWP is the most significant impact indicator according to Zhang et al.,¹¹ the GWP is analyzed in more detail. In addition, all results concerning the GWP are shown in Table S23–S25 in Supporting Information subdivided according to the respective LCA phases. Table S23 illustrates the results of 1 to 10 MW PtM-AEL plants. Further, Tables S24 and S25 show the results of 1 to 10 MW PtM-PEM and 1 to 10 MW PtM-SOEC plants, respectively.

Furthermore, only the LCIA results of 1 MW PtM plants are analyzed since the results of 5 and 10 MW plants hardly differ from the results of the 1 MW PtM plants. The results just decrease slightly (see Figure S28–S30 in Supporting Information) mainly due to the assumed electricity demand that refers to the FU of 1 kg of SNG and is assumed for all plant sizes (see Table 1). This agrees with the LCIA results from a study published by Parra et al.,¹⁷ where the results between different PtM-PEM plant sizes also barely changed. However, the GWP results are analyzed for all PtM plant sizes due to their significance. Besides this, it should be taken into consideration that the comparability of LCA results of different studies is limited since different methods and assumptions have been applied for each study.⁴⁵

GWP Results. What can be seen in Table 3 is that the CO₂ equiv results of PtM-SOEC plants for the energy scenarios in

Table 3. Results of CO₂ Equiv with Environmental Credit

range of kg CO ₂ equiv with respect to the water electrolysis technology and energy scenarios considering the environmental credit (values in kg CO ₂ equiv)						
energy scenarios	AEL		PEM		SOEC	
2019	11.64	11.46	12.21	12.01	9.96	9.78
2030	8.52	8.23	8.96	8.65	7.41	7.10
2050	6.84	6.48	7.21	6.83	6.02	5.64
EE	−0.56	−1.20	−0.50	−1.16	−0.06	−0.72

2019, 2030, and 2050 are the lowest in comparison to the results of PtM-AEL and PtM-PEM systems. The reason is mainly because the assumed electricity consumption for the hydrogen production in the use phase makes a decisive contribution to the CO₂ equiv/kg SNG (see Figures 4–6), which is also affirmed by Sternberg and Bardow.²³ The results are in the range of 9.96 kg CO₂ equiv/kg SNG (biogas) and 9.78 kg CO₂ equiv/kg SNG (air) for the energy scenario in 2019.

However, higher values of PtM-SOEC plants result when applying the RE scenario in contrast to the other systems because of two reasons. On the one hand, the heat demand for hydrogen production, modeled with the process “heat, district, or industrial, other than natural gas” in Umberto+, has a significant share on the total CO₂ equiv. On the other hand, the higher electricity demand of PtM-AEL and PtM-PEM systems has a lower impact on the CO₂ equiv results due to the missing fossil fuels in the RE scenario that are the main drivers of the CO₂ equiv.

The CO₂ equiv results of PtM-PEM systems are the highest (except for the RE scenario) and in the range of 12.21 kg CO₂ equiv/kg SNG (2019, biogas) and 12.01 kg CO₂ equiv/kg SNG (2019, air). The higher values result primarily due to the higher electricity demand for the hydrogen production, as mentioned above. Moreover, the PtM-AEL results are in the range of 11.64 kg CO₂ equiv/kg SNG (2019, cement) and 11.46 kg CO₂ equiv/kg SNG (2019, air). Besides that, PtM-PEM and PtM-SOEC

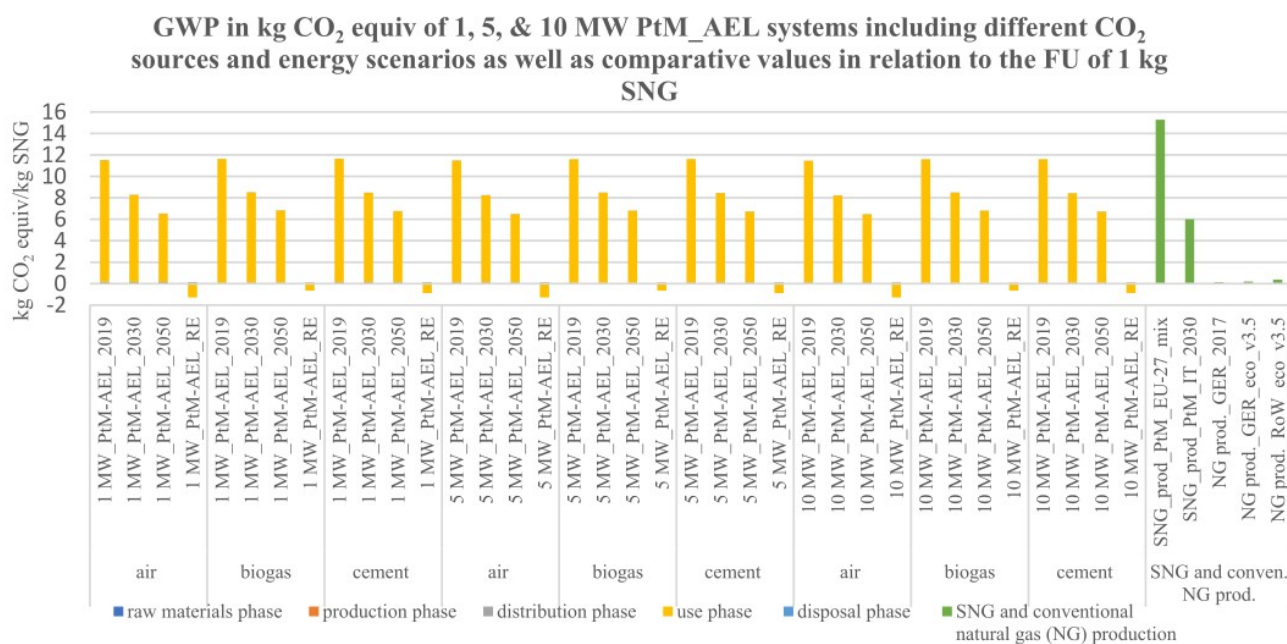


Figure 4. GWP results of PtM-AEL plants.

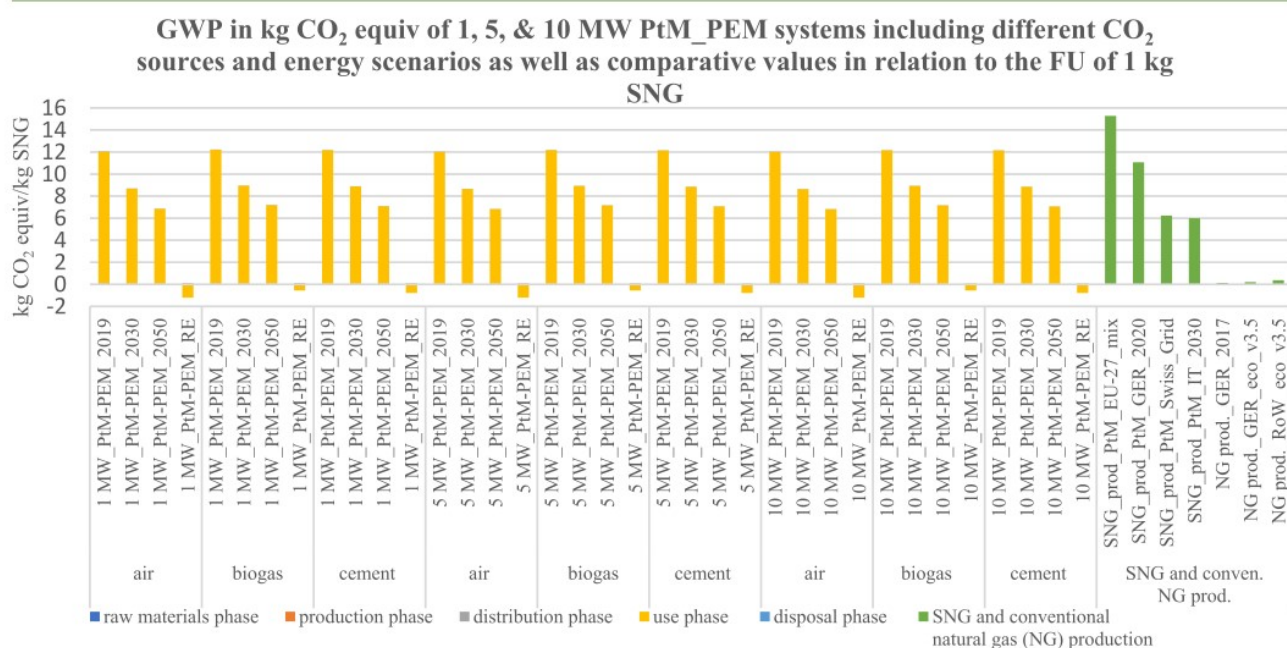


Figure 5. GWP results of PtM-PEM plants.

have the highest values with biogas as the CO₂ source, while this applies to PtM-AEL with cement as the CO₂ source.

The decrease of the CO₂ equiv in the use phase (see Figures 4–6) in between scenario 2019 and 2030 is in the range of 27.5–28.4% (air), 25.8–27% (biogas), and 26.3–27.3% (cement) considering all PtM systems. Moreover, the reduction of the CO₂ equiv in scenario 2050 compared to 2019 is in the range of 42.5–43.8% (air), 39.8–41.5% (biogas), and 40.5%–42.1% (cement). The main factor for the decline of the CO₂ equiv from 2019 to 2030 is due to the lower share of lignite and hard coal in the energy mix that decreased by 15.4% from 29.3% (2019) to 13.9% (2030). The removal of lignite and hard coal from the

energy mix in 2050 is the main factor for the reduction of the CO₂ equiv, even if the share of NG in the energy mix has almost doubled. Negative results for the RE scenario emerge regarding the CO₂ equiv since the environmental credit of -2.74 kg CO₂/kg SNG is considered and subtracted from the results (see Table 3).

What can be seen from the results in Tables S23–S25 (column “production phase”) is that the production phase considering the added manufacturing energy has only a very little impact on the overall results. Therefore, the potential environmental impacts of the added manufacturing energy are very small. Moreover, the results of the raw material,

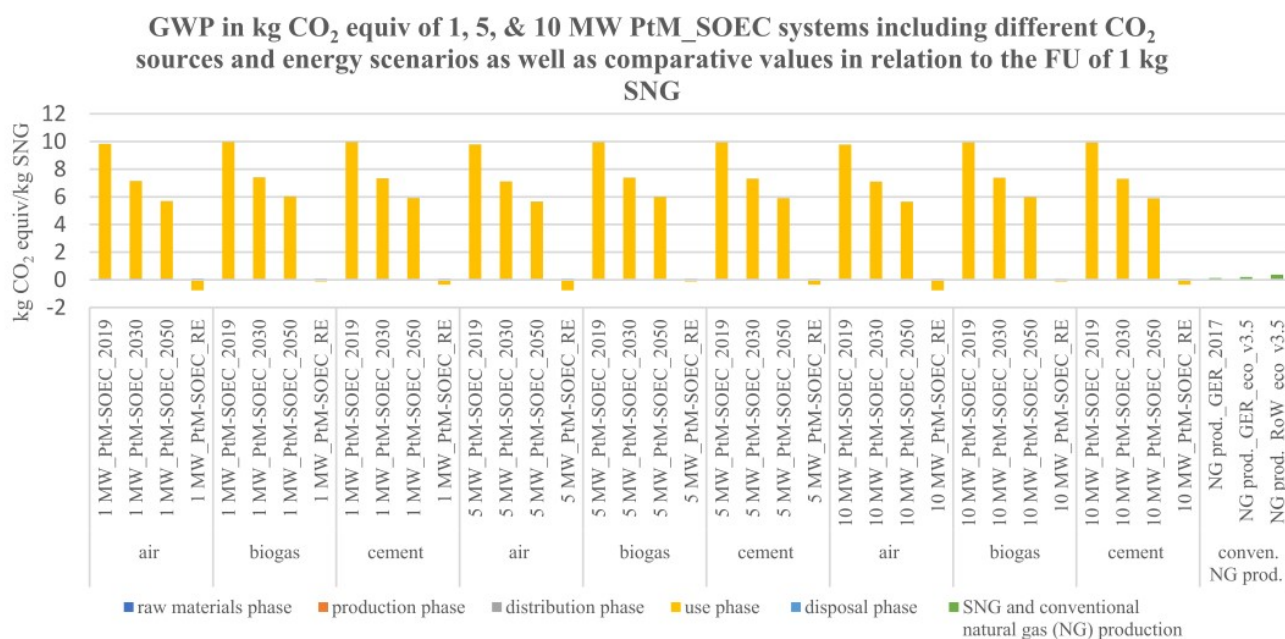


Figure 6. GWP results of PtM-SOEC plants.

distribution, and disposal phase have only a very small impact on the overall results as well (see Figures 4–6).

GWP Comparison with Other Studies and Conventional NG Production. As mentioned above, the comparison of the results with other LCA studies is limited. Nevertheless, the results are compared with values of other LCA studies for classification purposes.

The CO₂ equiv results of PtM-AEL and PtM-PEM plants are significantly smaller as the value published by Lindorfer/Reiter that is converted from 276 g CO₂ equiv/MJ to 15.29 kg CO₂ equiv/kg SNG through the higher heating value (HHV) of 55.4 MJ/kg CH₄ (see Figures 4–5).^{22,51} The value relates to PtM systems with AEL and PEM electrolyzers, whereby the CO₂ emissions have been regarded as waste and the EU-27 mix for electricity generation has been applied. The difference in relation to the value is mostly due to the environmental credit of -2.74 kg CO₂ equiv/kg SNG as well as using the HHV for the conversion of the value.

Moreover, the value published by Bargiacchi et al. for the base-case scenario of PtM-AEL and PtM-PEM plants is approx. 6 kg CO₂ equiv/kg SNG using a FU of 1 kg of SNG and a scenario of the Italian energy mix in 2030 with a high share of NG (38.5%), PV (24.3%), hydro (16.1%), and wind (13.1%) power.⁵² The value is within the lower range of the results of PtM-AEL and PtM-PEM plants by applying the energy scenario in 2050 (see Figures 4–5). The renewable energy (RE) share of 60.9% in the Italian energy mix corresponds roughly to the RE share (60%) in the energy scenario 2050. Moreover, the NG share of 38.5% (Italian energy mix) and 40% (2050's scenario) is also similar. These are the main reasons for similar results.

The 2019 results of PtM-PEM plants are above the value of approx. 11.07 kg CO₂ equiv/kg SNG according to Sternberg/Bardow taking a PEM electrolyzer and the forecasted energy mix in 2020 (Germany) into account (see Figure 5).²³ The original value corresponds to 0.222 kg CO₂ equiv/FU, whereas the FU consists of two parts (0.049 kWh for electricity generation and 1 MJ for SNG production).²³ Along with the information that 10% of the total kg CO₂ equiv has been assigned to the electricity

generation and 90% to the electrolysis for SNG production, 90% of the CO₂ equiv has been considered for the following estimation of the value (0.222 kg CO₂ equiv/FU times 0.9 equals to approx. 0.2 kg CO₂ equiv/MJ SNG times 55.4 MJ/kg CH₄ (HHV) corresponds to around 11.07 kg CO₂ equiv/kg SNG).²³

The value published by Parra et al. of 406 kg CO₂ equiv/MWh SNG that has been converted with a factor of 65 in kg SNG (assuming the HHV of 15.4 kWh/kg CH₄, thus dividing the FU of 1000 kWh by 15.4 kWh⁵¹) corresponds to approx. 6.24 kg CO₂ equiv/kg SNG.¹⁷ This value refers to a 1 MW PtM-PEM plant, where the CO₂ is derived from air. The value is in the range of 2050's PtM-PEM results (see Figure 5) primarily because the Swiss energy mix used in the study consists of a high share of hydro (60%) as well as nuclear power (33%) and, therefore, has a similar share of renewables in the energy mix.⁵³ The PtM-SOEC CO₂ equiv results are only compared with the values of the conventional NG production (see Figure 6) since no other comparative values were available.

The comparative values of the conventional NG production are in the range of 0.136 and 0.37 kg CO₂ equiv/kg NG. The value of 0.136 kg CO₂ equiv/kg NG refers to the NG production in Germany and is based on own calculations using published data,^{54,55} while the other values of 0.2 kg CO₂ equiv/kg NG and 0.37 kg CO₂ equiv/kg NG have been simulated with the Umberto + software. These values refer to Germany (0.2 kg CO₂ equiv/kg NG) and the RoW (0.37 kg CO₂ equiv/kg NG), respectively. Moreover, the calculated and modelled values for Germany are close to each other, while the value for the RoW (0.37 kg CO₂ equiv/kg) is almost three times and nearly twice as high as the values for Germany. In comparison with the value of 0.2 kg CO₂ equiv/kg NG, the CO₂ equiv results of the SNG production are approx. 61 times higher (2019) and up to 6 times lower (RE) than the comparative value. In summary, the conventional NG production is more attractive in terms of the CO₂ equiv than the SNG production when applying the energy scenarios in 2019, 2030, and 2050. This, however, does not

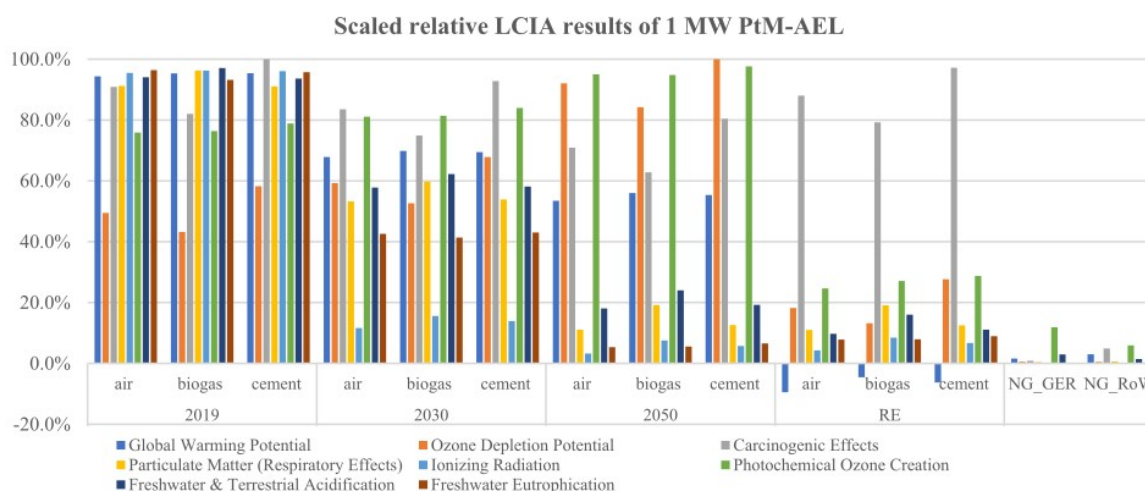


Figure 7. Scaled relative LCIA results of 1 MW PtM-AEL.

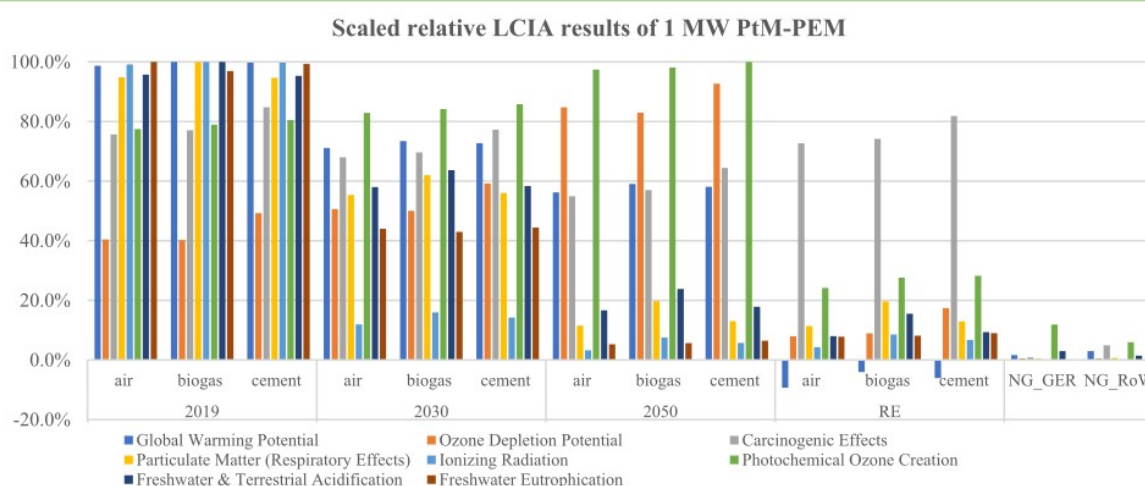


Figure 8. Scaled relative LCIA results of 1 MW PtM-PEM.

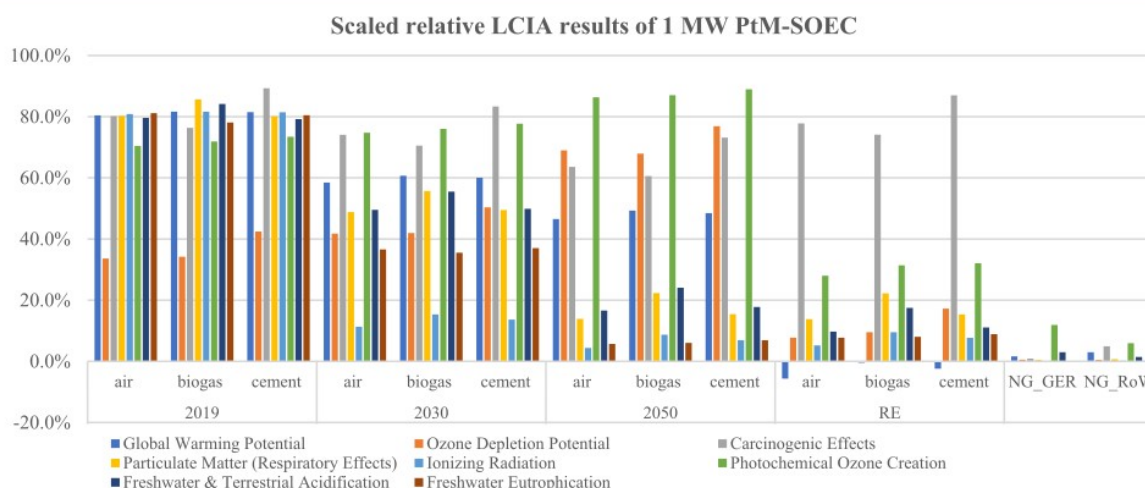


Figure 9. Scaled relative LCIA results of 1 MW PtM-SOEC.

apply to the RE scenario due to the environmental credit and the resulting negative values (see Table 3).

LCIA Results of 1 MW PtM Plants. The results of the LCIA indicators are discussed in this section. The GWP, that has been

analyzed in detail previously, is not part of the discussion. Nevertheless, the indicator has been considered for comparison purposes; thus, the results are depicted in Figures 7–9. To scale the relative LCIA results, the values shown in Table 4 have been

Table 4. Maximum Values of the LCA Indicators

PtM technology	CO ₂ source	energy scenario	abbreviation	main drivers	value	unit per kg SNG
PtM-PEM	biogas	2019	GWP	electricity production lignite coal	1.22×10^1	kg CO ₂ equiv
PtM-AEL	cement	2050	ODP	electricity production NG	2.10×10^{-6}	kg CFC-11 equiv
PtM-AEL	cement	2019	CE	electricity production lignite coal	1.39×10^{-7}	CTUh
PtM-PEM	biogas	2019	PM	electricity production biogas burned	1.11×10^{-6}	disease incidences
PtM-PEM	biogas	2019	IR	electricity production nuclear	3.16	kg ^{U235} -equiv
PtM-PEM	cement	2050	POC	electricity production NG	2.83×10^{-2}	kg NMVOC-equiv
PtM-PEM	biogas	2019	Acid.	electricity production biogas burned	1.75×10^{-1}	mol H ⁺ -equiv
PtM-PEM	air	2019	Eutr.	electricity production lignite coal	2.01×10^{-2}	kg P-equiv

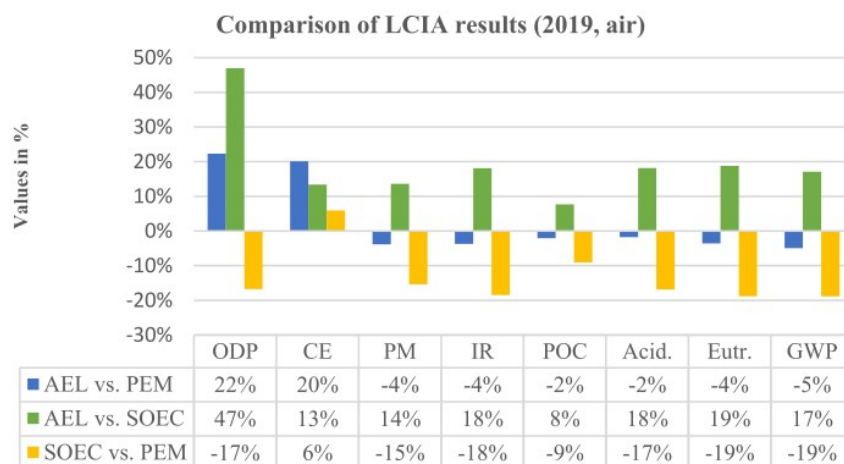


Figure 10. Comparison of the LCIA results applying the energy scenario of 2019 (air).

used. These values are the maximum values of the chosen indicators. Furthermore, the LCIA indicators are described, and the main reasons for the change in the results are analyzed. Thereafter, the results—including the GWP—are compared with each other to analyze which PtM technology is potentially the most environmentally friendly one for the respective energy scenario. Further, a comparison with results of other LCA studies is carried out.

LCIA Indicators (Maximum Values). Table 4 shows the maximum values of the LCIA indicators. The maximum values for GWP, particulate matter (PM) (respiratory effects), ionizing radiation and freshwater and terrestrial acidification are related to the 1 MW PtM-PEM plant, where the energy scenario in 2019 and biogas as the CO₂ source are used (2019, biogas). Moreover, the maximum values for photochemical ozone creation and freshwater eutrophication are assigned to 1 MW PtM-PEM (2050, cement) and 1 MW PtM-PEM (2019, air), respectively. Further, the highest values for carcinogenic effects and ozone depletion potential (ODP) relate to 1 MW PtM-AEL (2019, cement) and 1 MW PtM-AEL (2050, cement), respectively.

The maximum values of the PtM-PEM systems result primarily due to the higher electricity consumption. This applies also to the PtM-AEL maximum values, even though the chromium steel (carcinogenic effects) and tetrafluoroethylene production (ODP) processes have an enormous impact on the results as well.

Description and Discussion of the LCIA indicators and the Main Reasons of the Change in the Results. The ODP indicator represents the ozone depletion potential.^{49,56} The indicator rises from 2019 to 2050 by more than 30%—considering all PtM systems—primarily due to electricity

production from NG and the fact that the share has almost doubled in 2050's energy scenario (see Figure 3). The ODP results decline considerably when applying the RE scenario mostly due to the missing NG in the energy mix. Since ozone filters the ultraviolet B (UVB) radiation and protects human beings and plants against sun rays, the ozone depletion has a negative impact on human health and plants.

The carcinogenic effect indicator, which is given in the unit comparative toxic unit for humans (CTUh), estimates the potential increase of disease cases per kilogram of a substance emitted.⁴⁹ The results of the carcinogenic effects fall by more than 15% from 2019–2050 mainly due to the decline of lignite coal in the energy mixes. However, the results increase by more than 13% in the RE scenario mostly because of the higher share of wind energy (onshore) in the energy mix.

The indicator PM (respiratory effects), measured in disease incidences/kg PM_{2.5}, relates to fine dust emissions and shows potential impacts on human health.⁵⁰ In particular, particles smaller than 10 μm are responsible for effects on human health, such as heart and lung diseases.⁵⁷ For all PtM systems, the indicator sinks significantly from 2019 to the RE scenario by more than 60%. The decline of biomass, particularly burned biogas, is the main cause of this decrease.

In addition, the ionizing radiation indicator drops considerably from 2019 to 2030 by more than 65% due to the phase-out of nuclear power. Ionizing radiation can create various cancer types as well as affect the DNA.⁴⁹

Furthermore, the photochemical ozone creation indicator rises from 2019 to 2050, while the indicator falls significantly by more than 55% in the RE scenario. The main driver for the decline is NG that is not present in the RE energy scenario anymore. Tropospheric ozone (summer smog) can be created

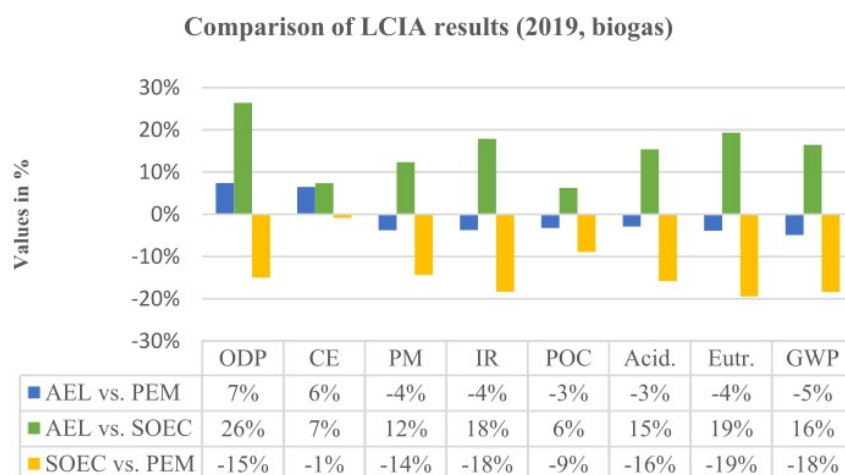


Figure 11. Comparison of the LCIA results applying the energy scenario of 2019 (biogas).

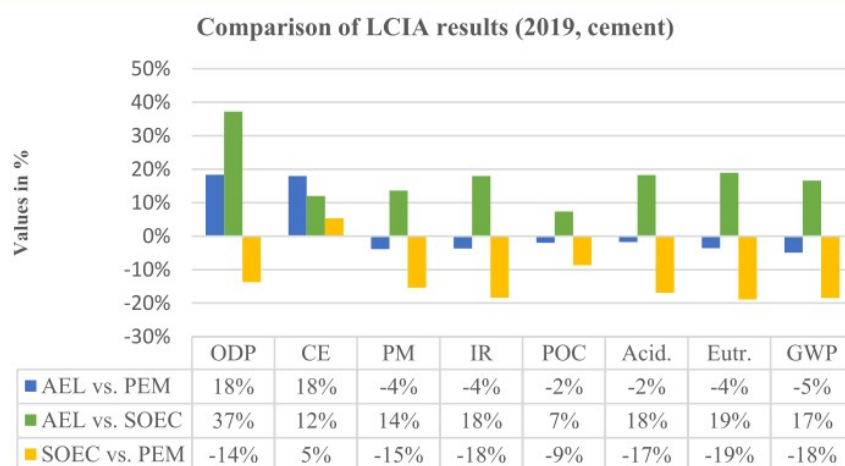


Figure 12. Comparison of the LCIA results applying the energy scenario of 2019 (cement).

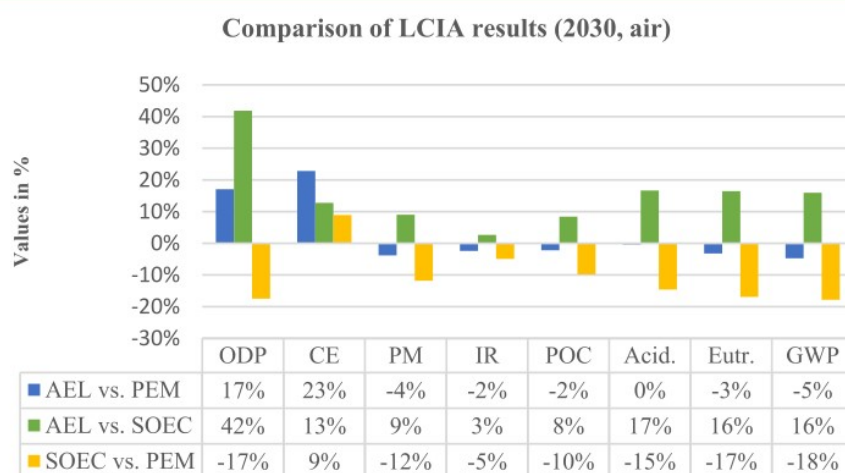


Figure 13. Comparison of the LCIA results applying the energy scenario of 2030 (air).

by photochemical ozone and affect human health in relation to heart and lung problems.^{49,58}

Due to the decline of biomass in the energy mixes, the freshwater and terrestrial acidification indicator decreases

constantly from 2019 to 2050. The indicator shows the potential acidification of soil and freshwater.⁵⁰

The indicator freshwater eutrophication declines considerably from 2019 to 2050 by more than 70%. The main reason is the decrease of lignite and hard coal to zero percent in the energy

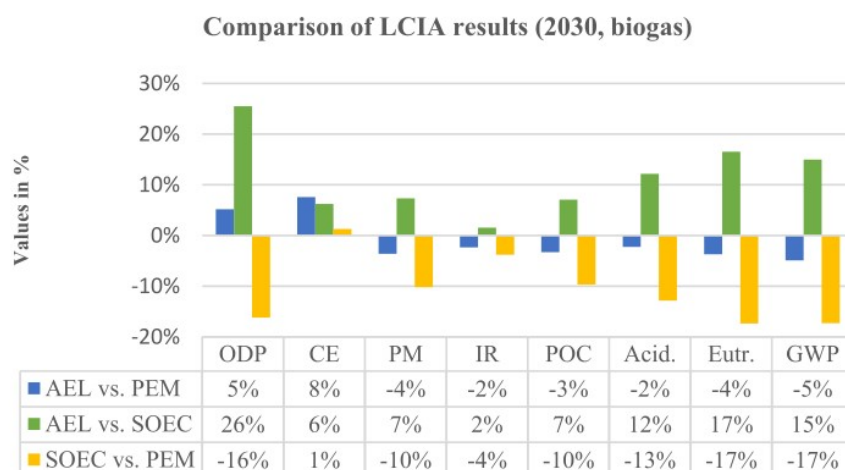


Figure 14. Comparison of the LCIA results applying the energy scenario of 2030 (biogas).

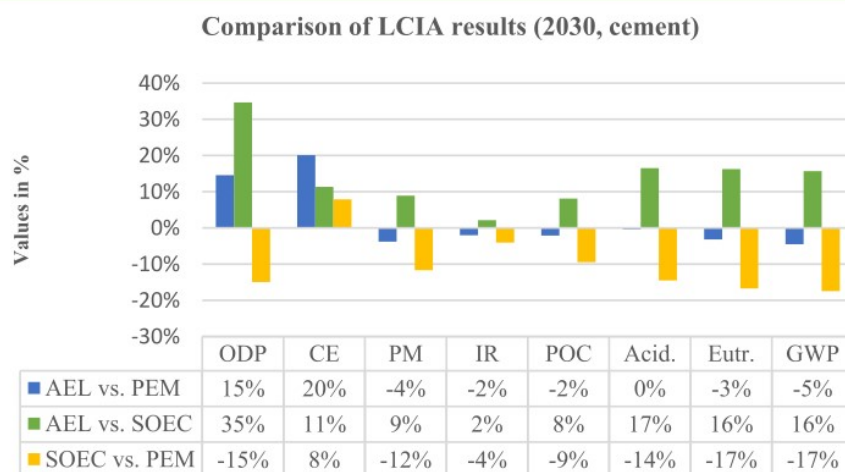


Figure 15. Comparison of the LCIA results applying the energy scenario of 2030 (cement).

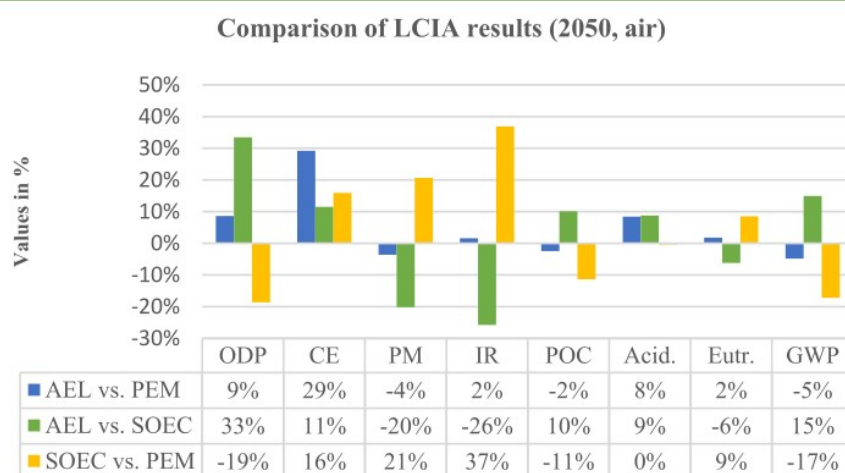


Figure 16. Comparison of the LCIA results applying the energy scenario of 2050 (air).

mix in 2050. The indicator considers only phosphorus emissions and shows the potential environmental impacts on rivers and lakes mostly caused by a surplus of nutrients.⁴⁹

Also, what can be seen in Figures 7–9 is that the values of the LCIA indicators (except GWP) are above the potential

environmental impacts of the conventional NG production in Germany and the RoW. Thus, the conventional NG production is potentially more environmentally friendly than the SNG production considering all applied energy scenarios.

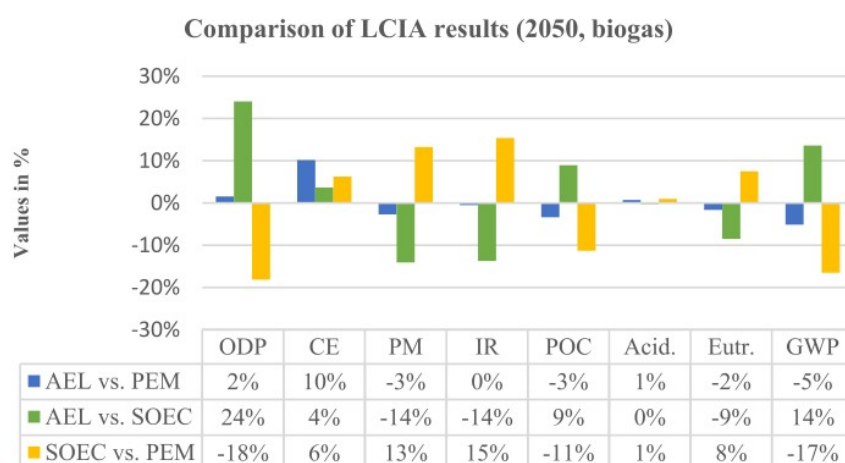


Figure 17. Comparison of the LCIA results applying the energy scenario of 2050 (biogas).

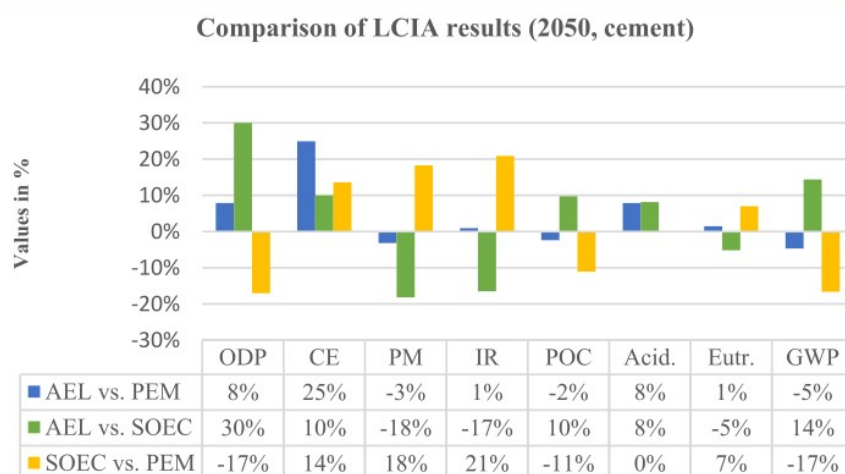


Figure 18. Comparison of the LCIA results applying the energy scenario of 2050 (cement).

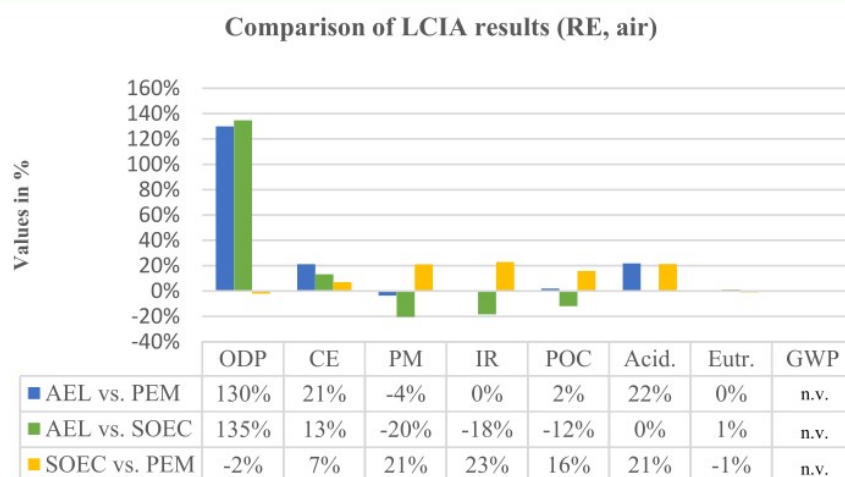


Figure 19. Comparison of the LCIA results applying the RE scenario (air).

Comparison of 1 MW PtM Results. In this section, the 1 MW PtM results are compared with each other considering the GWP and the previously analyzed LCIA indicators (see Figures 10–21). For the comparison, all LCIA indicators are weighted equally.

The results are attached in [Supporting Information Section 8](#), where the maximum values of the compared LCIA indicators are marked in red, and the minimum values are marked in green. To understand the interpretation of the results in Figures 10–21, the following example is shown using the first graph (see [Figure](#)

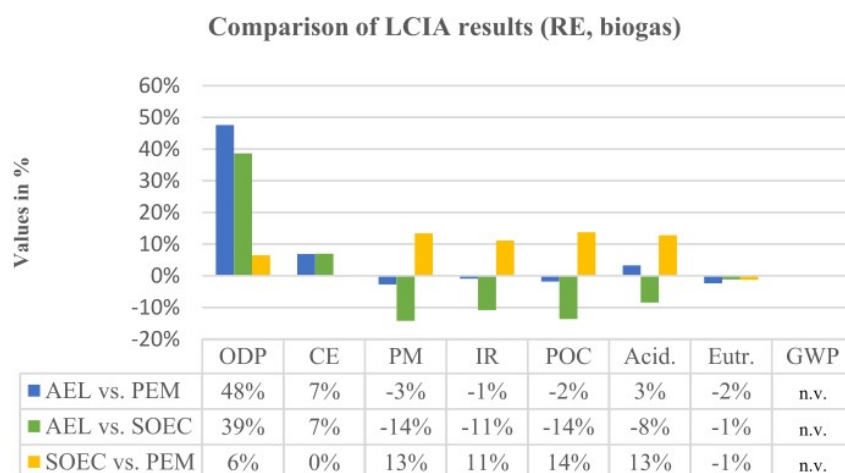


Figure 20. Comparison of the LCIA results applying the RE scenario (biogas).

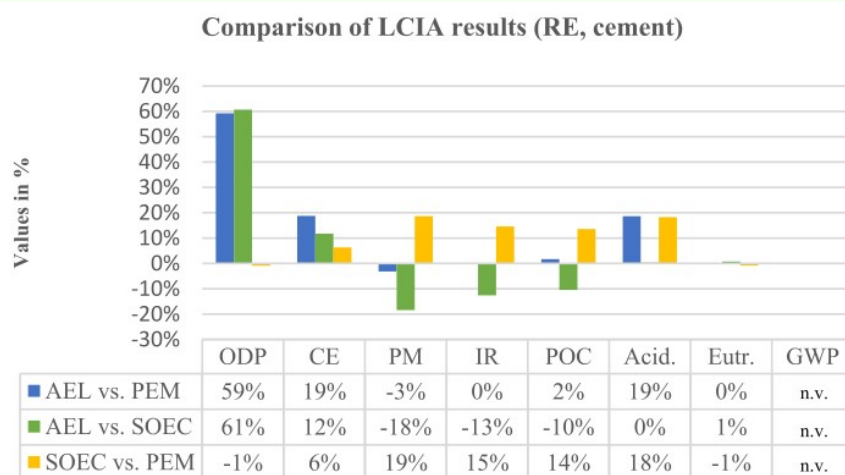


Figure 21. Comparison of the LCIA results applying the RE scenario (cement).

10). The ODP result for PtM-AEL is 22% higher in comparison with PtM-PEM. Thus, the potential environmental impact of PtM-PEM is lower regarding the ODP and PtM-PEM is preferable to PtM-AEL. Regarding a negative value, the opposite interpretation applies. PtM-AEL shows a negative value of -4% compared to PtM-PEM concerning PM. This means that PtM-PEM has a higher potential environmental impact; thus, PtM-AEL is preferable to PtM-PEM. This process of evaluation has been applied in the subsequent discussion of the results.

PtM-SOEC plants show the lowest potential environmental impacts for seven out of eight LCIA indicators—except for the 2019 biogas scenario, where all eight indicators are the lowest—considering the energy scenarios in 2019, 2030, and all CO₂ sources. Thus, PtM-SOEC has potentially the most environmentally friendly technology in comparison to PtM-AEL and PtM-PEM when applying the energy scenarios in 2019 and 2030. Moreover, PtM-AEL shows the highest results in terms of carcinogenic effects and ODP because of the chromium steel production process (carcinogenic effects)—due to the higher steel demand for the stack—and the tetrafluoroethylene production process for the gasket (ODP). The results of the other LCIA indicators are in between the values of PtM-SOEC and PtM-PEM for the energy scenarios in 2019 and 2030.

Further, six out of eight maximum values of the LCIA indicators are assigned to PtM-PEM plants for the energy scenarios in 2019 and 2030 primarily due to the higher electricity demand for the SNG production. However, the maximum values of the six indicators differ only slightly from the PtM-AEL results. Consequently, PtM-AEL can be described as potentially the most environmentally unfriendly technology for the respective energy scenarios with air and cement as the CO₂ source due to the significantly higher values for carcinogenic effects and ODP. Regarding the energy scenario in 2019 and 2030 with biogas as the CO₂ source, the results between PtM-PEM and PtM-AEL do not differ a lot.

The 2050 results of PtM-PEM with air and cement as the CO₂ sources are at a similar level in comparison to PtM-AEL, except for the indicator carcinogenic effects that is considerably higher for PtM-AEL. Moreover, the results of PtM-PEM concerning the carcinogenic effects, PM and ionizing radiation are significantly lower compared to PtM-SOEC, while the results for ODP, photochemical ozone creation, and GWP are much higher. For freshwater and terrestrial acidification and freshwater eutrophication, nearly similar values result. Overall, PtM-PEM with air and cement as the CO₂ source is potentially more environmentally friendly than PtM-AEL and PtM-SOEC when applying the energy scenario in 2050. However, no clear

statement can be made regarding the results considering the energy scenario in 2050 and biogas as the CO₂ source since the results in total hardly differ from each other.

Furthermore, PtM-PEM can be seen as potentially the most environmentally friendly technology for the RE scenario taking all CO₂ sources into account since the results of PM, ionizing radiation, photochemical ozone creation, and freshwater and terrestrial acidification are significantly lower compared to the results of PtM-SOEC. This applies in comparison to PtM-AEL with air and cement as the CO₂ sources to the indicators ODP, carcinogenic effects, and freshwater and terrestrial acidification. For the comparison of PtM-PEM with PtM-AEL and biogas as the CO₂ source, only the ODP indicator shows an extreme deviation, while the other results are close to each other. Moreover, PtM-AEL can be classified as potentially more environmentally harmful than PtM-SOEC for the RE scenario because of the ODP indicator. However, without considering the ODP indicator, PtM-SOEC can be seen as potentially the most environmentally harmful technology for the RE energy scenario.

Comparison with Other Studies. As mentioned earlier, there are hardly any comparison values of LCIA indicators available due to the fact that only a few studies have been conducted regarding the topic. Moreover, these values are limited for comparison purposes since different scenarios and methods have been applied in the studies. However, a rough classification of the results published by Parra et al.¹⁷ and Bargiacchi et al.⁵² is carried out. The values by Parra et al. have been converted using a factor of 65 (as described above), while the values by Bargiacchi et al. have not been modified since they relate to the FU of 1 kg of SNG.

The values for PM and ionizing radiation for a 1 MW PtM-PEM plant considering air as the CO₂ are far above the results in Table S29 (see Supporting Information). These values were published by Parra et al. in 2017 taking the Swiss wholesale market electricity supply with a high share of hydropower (approx. 60%) into account.^{17,53} The main reason is that hydropower, pumped storage, contributes considerably to the PM results (modeled with Umberto+). On the other hand, the electricity production from nuclear power plants is the main driver for ionizing radiation, and the Swiss energy mix consists of approx. 33% nuclear power.⁵³ Furthermore, the LCIA indicator carcinogenic effects were not under study. The value for ODP is similar to 2030's results. Further, the values for photochemical ozone creation and freshwater and terrestrial acidification are lower than 2019's, 2030's, and 2050's results, however, higher than the RE scenario results. The value for freshwater eutrophication is lower than 2019's and 2030's results and higher than the 2050's and the RE scenario results. In summary, the RE scenario results are more environmentally friendly than the values published by Parra et al.¹⁷ because it consists only of renewables (wind and solar energy); thus, it has no share of fossil fuels. In addition, it is noticeable that the values for PM and ionizing radiation deviate significantly from the values in this study due to the Swiss energy mix and the large extent of hydro and nuclear power.

In comparison to the study by Bargiacchi et al. that analyzed PtM-AEL and PtM-PEM plants with CO₂ delivered from various point sources,⁵² the base-case values for PM and carcinogenic effects are higher than the results in Table S30 and S31 (see Supporting Information). Furthermore, the base-case value for freshwater eutrophication is lower, while the result for ionizing radiation is close to 2050's results of PtM-AEL and

PtM-PEM plants with air as the CO₂ source. Moreover, the base-case result of the ODP indicator is in the range of 2030's values. The photochemical ozone creation base-case result is higher than the values of the RE scenario, however, smaller than the results of the other scenarios. Further, the value for freshwater and terrestrial acidification is lower than 2019's and 2030's results, however, higher than 2050's and the RE scenario results.

Because a comparison of LCA results is difficult, as stated above, and the lack of information that is necessary to compare the results in more detail, a deeper analysis of the results could not be carried out.

Utilization of SNG as Electricity or Fuel (Scenario 2). In the second scenario, it is assumed that the produced SNG is used for electricity generation and as a fuel for cars without considering the environmental credit since the bonded CO₂ is released into the atmosphere through the conversion processes. Thus, the following values result (see Table 5).

Table 5. CO₂ Equiv without Environmental Credit

range of kg CO ₂ equiv with respect to the water electrolysis technology and energy scenarios without considering the environmental credit (values in kg CO ₂ equiv)						
energy scenarios	AEL		PEM		SOEC	
2019	14.38	14.20	14.95	14.75	12.70	12.52
2030	11.26	10.97	11.70	11.39	10.15	9.84
2050	9.58	9.22	9.95	9.57	8.76	8.38
RE	2.18	1.54	2.24	1.58	2.68	2.02

With respect to the utilization of SNG for electricity generation, the values in Table 6 (in kg of CO₂ equiv/kWh)

Table 6. Results of CO₂ Equiv per Kilowatt Hour

range of kg CO ₂ equiv per kWh with respect to the water electrolysis technology and energy scenarios (values in kg CO ₂ equiv/kWh)						
energy scenarios	AEL		PEM		SOEC	
2019	0.934	0.922	0.971	0.958	0.825	0.813
2030	0.731	0.712	0.760	0.740	0.659	0.639
2050	0.622	0.599	0.646	0.621	0.569	0.544
RE	0.142	0.100	0.145	0.103	0.174	0.131

emerge, assuming that approx. 15.4 kWh (HHV) can be generated from 1 kg of CH₄ (SNG).⁵¹ However, the combustion process itself, converting SNG into electricity, has not been considered since it just has a slight impact on the results.

To classify the results, Figure 22 shows comparative values for electricity generation in kg CO₂/kWh from lignite and hard coal as well as from NG and the German energy mix in 2019. The comparative values are derived from refs 59 and 60.

The results are below the comparison values of lignite and hard coal, and thus, they cause less potential environmental impacts than these. Furthermore, 2050's results are one-third lower than 2019's results due to the missing shares of lignite and hard coal in the energy mix, even if the natural gas share has increased from 21.2 to 40%. Moreover, the results decrease sharply from 2019's scenario to the RE scenario, making this scenario the most environmentally friendly one for the electricity generation from SNG in comparison to the conventional alternatives since no fossil fuels are included in the energy mix anymore. Therefore, the SNG produced by the RE scenario enables a greener electricity production compared to the conventional one, thus having an enormous potential to

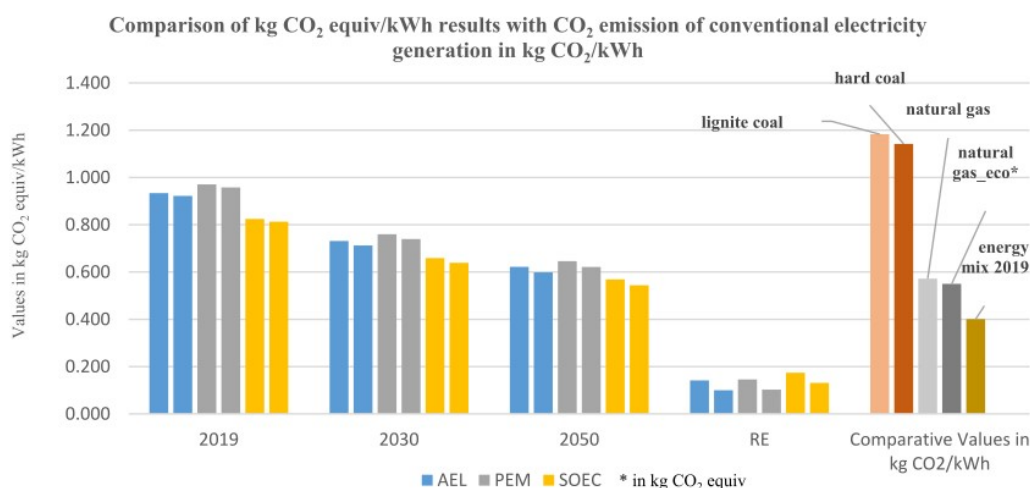


Figure 22. Comparative values concerning conventional electricity generation.

reduce CO₂ emissions and mitigate climate change. The electricity generation from green-produced SNG offers a climate-friendly opportunity. However, the energy transition needs to accelerate considerably for this.

Regarding the utilization of SNG as a fuel for cars, the results in Table 7 (in g CO₂ equiv/km) emerge, assuming that 1 kg

Table 7. Results of CO₂ Equiv per Kilometer

range of g CO ₂ equiv per km with respect to the water electrolysis technology and energy scenarios (values in g CO ₂ equiv/km)						
energy scenarios	AEL		PEM		SOEC	
2019	737.4	728.2	766.7	756.4	651.3	642.1
2030	577.4	562.6	600.0	584.1	520.5	504.6
2050	491.3	472.8	510.3	490.8	449.2	429.7
RE	111.8	79.0	114.9	81.0	137.4	103.6

SNG as a fuel has a range of 19.5 km by car. The following calculation has been done concerning the value of 19.5 km: 1 kg SNG divided by 0.668 kg/Nm³ CH₄ equals around 1.5 Nm³ of SNG that is further multiplied with a factor of 0.076693 Nm³ CH₄/km according to Zhang et al.⁴⁶ This corresponds to approx. 19.5 km. The results are significantly higher than the

comparative values when applying the energy scenarios in 2019, 2030, and 2050 (see Figure 23).⁶¹ Thus, only the results of the RE scenario are competitive with the conventional fuels. These results are lower than the values for petrol, diesel, and liquefied petroleum gas (LPG). Moreover, the results of PtM-AEL and PtM-PEM, both with air as the CO₂ source, are lower than the value of compressed natural gas (CNG). Hence, only the SNG produced by the RE scenario is an attractive alternative compared to the conventional fuels and has the potential to help reduce CO₂ emissions, with regard to petrol, diesel, and LPG.

In summary, only the SNG produced by the RE scenario is appropriate for electricity generation or as a fuel for cars compared to conventional alternatives. Thus, the green-produced SNG can help reduce CO₂ emissions, mitigate climate change, and reach the government's goal by 2040.

Note that the CO₂ emissions of the conventional alternatives have been compared with potential CO₂ equiv (see Figures 22 and 23). The CO₂ equiv consists of other substances, such as methane. To draw a more realistic comparison, the CO₂ emissions of the conventional alternatives have been considered instead of the modeled values with Umberto+ (both the CO₂

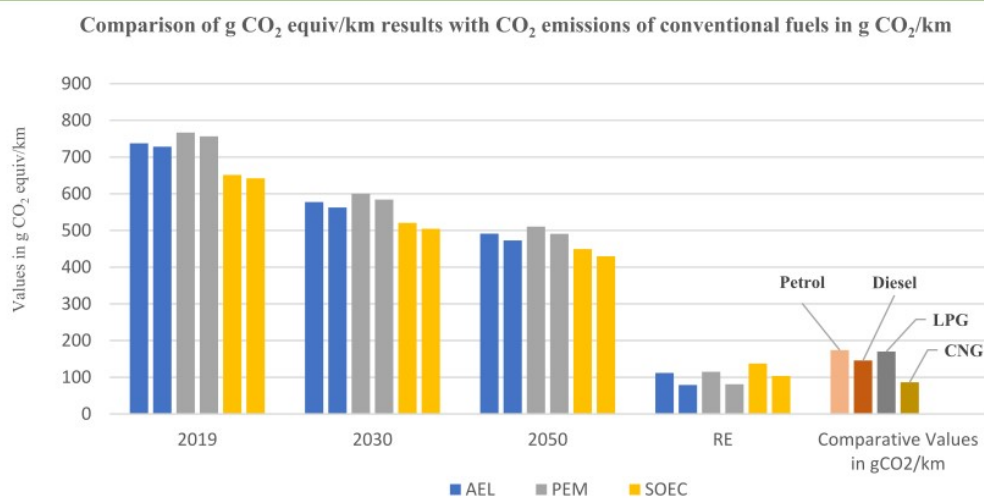


Figure 23. Comparative values concerning conventional fuels.

emissions and the Umberto+ values are shown in Tables S32 and S33 in Supporting Information for comparison purposes). The reason is that the values in g CO₂/km and the Umberto + values in g CO₂ equiv/km differ significantly becauseecoinvent considered additional processes that lead to higher values, such as car production and maintenance of infrastructure processes. On the other hand, the Umberto+ results in kg CO₂ equiv/kWh and the CO₂ emissions in kg CO₂/kWh hardly differ from each other (see Supporting Information Table S32 and S33).^{59–61}

Future Work. Concerning future work, the conversion process of SNG into electricity will be considered as well as the car production process regarding the utilization of SNG as a fuel for cars.

CONCLUSIONS

In this study, the potential environmental impacts of a greener SNG production, particularly the CO₂ equiv, have been analyzed. For this, different water electrolysis technologies (AEL, PEM, and SOEC), CO₂ sources (air, biogas, and cement plant) and energy scenarios (2019, 2030, 2050, and RE) with an increasing share of wind and solar energy have been considered to depict a greener SNG production. Regarding this, two scenarios have been created. The first scenario comprises the SNG production for storage purposes in the natural gas grid including an environmental credit of −1 kg CO₂/kg CO₂ since the CO₂ is withdrawn from the atmosphere and bonded in the SNG. The aim was to analyze which PtM technology shows the lowest CO₂ equiv and which is potentially the most environmentally friendly one for the respective energy scenario considering all indicators. Furthermore, the results have been compared to the potential environmental impacts of conventional natural gas production. In the second scenario, the produced SNG has been contemplated for electricity generation and as a fuel for cars to compare the resulting CO₂ equiv with the CO₂ emissions of conventional electricity generation and conventional fuels for cars. The study concludes that PtM-SOEC shows the lowest CO₂ equiv for the energy scenarios in 2019, 2030, and 2050. This applies to PtM-AEL regarding the RE scenario. Furthermore, PtM-SOEC is potentially the most environmentally friendly technology for the energy scenarios in 2019 and 2030 taking all indicators into account. This applies to PtM-PEM for both the energy scenarios in 2050 (with air and cement as CO₂ sources) and the RE scenario; however, no clear statement can be made regarding the energy scenario in 2050 with biogas as the CO₂ source. Hence, SNG production is recommended for the energy scenarios in 2019 and 2030 with the PtM-SOEC technology, while this applies to the PtM-PEM technology for the energy scenario in 2050 and the RE scenario. Thus, a more environmentally friendly SNG production can be implemented to keep the potential environmental impacts as low as possible. Moreover, the conventional NG production shows less potential environmental impacts than the SNG production considering all energy scenarios. In comparison to the CO₂ emissions of the conventional electricity generation and the conventional fuels for cars, only the SNG produced by the RE energy scenario shows results that are below the comparative values (except for CNG). Therefore, merely energy mixes with a very high share of wind and solar energy are appropriate for a greener SNG production. Then, greener-produced SNG is an attractive alternative in comparison to the conventional ones and can help minimize environmental impacts, particularly CO₂ emissions. For this, the energy transition in Germany regarding wind and solar energy is essential because the share in 2019's

energy mix is only around 33%. Thus, the expansion of wind and solar energy in the future holds the opportunity of a greener SNG production and the replacement of conventional alternatives. Although the expansion of wind and solar energy leads to fluctuations in the electricity grid, they can, however, be compensated by the utilization of SNG for electricity generation, especially since the infrastructure of the natural gas grid as a flexible storage location is already in place, and the capacity is sufficient. The stored SNG can then be used at any time to compensate for fluctuations in the grid. Besides this, the expansion of wind and solar energy along with a greener SNG production can help to achieve the target of the federal government of Germany, to reduce CO₂ emissions by 88% by 2040, and minimize global warming, thus supporting the Paris agreement.

Limitations. The limitations of the study are addressed in this section. Since there is a limited choice of material processes in the ecoinvent database, the materials LSM and iridium have been self-created considering the literature. For this reason, fewer potential environmental impacts could be depicted compared to basic ecoinvent processes due to the lack of information in the literature. However, the materials have just a little share of the mass balance; therefore, the impacts on the results are negligible. Besides this, hardly any recycling processes are available in the database for the disposal phase. Consequently, with a larger variety of recycling processes, for example, for copper and aluminum, the potential environmental impacts would have been lower because in some cases, a recycling process causes fewer environmental impacts than the extraction of the raw material, as with copper and aluminum. Nevertheless, the impacts of the disposal phase on the results are inconsiderable. Moreover, the data availability can be seen as a limitation, especially regarding the SOEC stack and BoP components. The reason is that the technology is still in the developing stage; therefore, hardly any data were accessible. The profound data generation, however, enables a great opportunity for further research projects.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acssuschemeng.1c02002>.

Description of the data generation, the results of the work, and values entered in the software Umberto+ (PDF)

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Notes

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■ ABBREVIATIONS

AD	outer diameter
AE	accumulated exceedance
AEL	alkaline electrolysis
APOS	allocation at point of substitution
BoP	balance of plant
CH	represents Switzerland in the ecoinvent database
CNG	compressed natural gas
DAC	direct air capture
DE	represents Germany in the ecoinvent database
DNA	deoxyribonucleic acid
eq	equation
EU	European Union
Fig.	figure
FU	functional unit
GLO	represents global in the ecoinvent database
GWP	global warming potential
HHV	higher heating value
ID	inner diameter
ILCD	International Life Cycle Data
IndWEDe	industrialisierung der wasserelektrolyse in Deutschland
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
LCA	life cycle assessment
LCI	life cycle inventory
LCIA	life-cycle impact assessment
LHV	lower heating value
LPG	liquefied petroleum gas
LSM	lanthanum–strontium–manganite
MEA	membrane electrode assembly
VNG	natural gas
ODP	ozone depletion potential
PEM	polymer-exchange membrane
PEMFC	polymer-exchange membrane fuel cell
PtG	power to gas
PtM	power to methane
PV	photovoltaic
RE	renewable energy
RER	represents Europe in the ecoinvent database
RoW	represents rest of the world in the ecoinvent database
SI	supporting information
SNG	synthetic natural gas
SOEC	solid-oxide electrolyzer cell
SOFC	solid-oxide fuel cell
Tab.	table
U.S.	United States
UVB	ultraviolet B rays
w/w	weight per weight
wt %	weight percent

■ CHEMICAL SUM FORMULA

CH ₄	methane
CO ₂	carbon dioxide
e ⁻	electron
H ₂	hydrogen
H ₂ O	water
H ₂ S	hydrogen sulfide

H ₃ O ⁺ /H ⁺	oxonium ion
KOH	potassium hydroxide
N ₂	nitrogen
NaOH	sodium hydroxide
O ²⁻	oxide ion
OH ⁻	hydroxide ion
Y ₂ O ₃	yttrium oxide
ZrO ₂	zirconium oxide

■ UNITS OF LCIA INDICATORS

CFC-11 equiv	trichlorofluoromethane equivalent, unit of ozone layer depletion
CO ₂ equiv	carbon dioxide equivalent, unit of global warming potential
CTUh	comparative toxic unit for humans, unit of carcinogenic effects
Mol H ⁺ -equiv	mol hydron equivalent, unit of acidification potential
NMVOC-equiv	nonmethane volatile organic compounds equivalents, unit of photochemical ozone creation
P-equiv	phosphor equivalent, unit of freshwater eutrophication
PM2.5	particulate matter less than 2.5 μm, unit of particulate matter
U ²³⁵ equiv	uranium-235 equivalent, unit of ionizing radiation

■ UNITS

A/cm ²	ampere per square meter
dm ³	decimeter
ft	foot
g	gram
GW	gigawatt
h	hour
kg	kilogram
km	kilometer
kW	kilowatt
kWh	kilowatt hour
l	litre
mH ₂ ³	cubic meter of hydrogen
MJ	megajoule
mm	millimeter
MW	megawatt
MW h	megawatt hour
N m ³	standard cubic meter
t	ton
TWh	terawatt hour
USD	US dollar
°C	degrees Celsius

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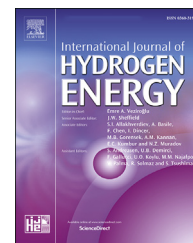
Abstract: The transformation to a greener energy system leads to new challenges, as wind and solar power are not always available. A solution for this challenge is the generation of synthetic natural gas (SNG) and hydrogen from (surplus) wind and solar power, so that the green gases can be stored in the natural gas grid long-term and be used for electricity generation when wind and solar power are not accessible. This solution is especially of interest if the storage infrastructure is already in place, as in Germany, since investment costs can be avoided. Because of that, the study investigates the levelized cost of SNG and hydrogen generation in Germany applying the cost estimation method by Rubin et al. For the investigation, different water electrolysis technologies (alkaline electrolysis, polymer exchange membrane, and solid oxide electrolyzer cell with a size of 1 and 100 MW) and energy scenarios (8,000h grid, 2,000h grid, wind, and solar) are contemplated. Besides that, the environmental costs of SNG and hydrogen generation in Germany are investigated due to the increasing importance of these costs for society and companies. The author concludes that the levelized costs of SNG and hydrogen are far too high compared to peer studies, as more cost factors have been considered after applying the method by Rubin et al. In terms of the environmental costs, the use of Germany's grid electricity is not recommended for SNG and hydrogen generation since the generation from wind and solar power is more environmentally friendly, whereby wind power is preferable over solar power.



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Levelized and environmental costs of power-to-gas generation in Germany

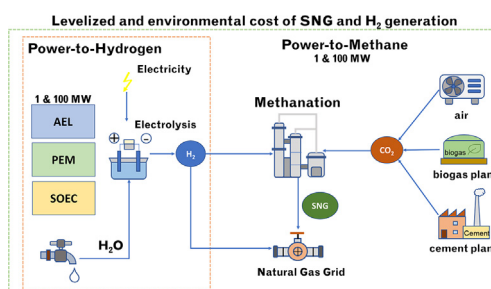
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HIGHLIGHTS

- The study shows a new perspective on levelized cost of SNG and H₂.
- The method by Rubin et al. leads to very high results compared to peer studies.
- Wind energy causes the lowest environmental costs of SNG and H₂ generation.

GRAPHICAL ABSTRACT



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ABSTRACT

The transformation to a greener energy system leads to new challenges, as wind and solar power are not always available. A solution for this challenge is the generation of synthetic natural gas (SNG) and hydrogen from (surplus) wind and solar power, so that the green gases can be stored in the natural gas grid long-term and be used for electricity generation when wind and solar power are not accessible. This solution is especially of interest if the storage infrastructure is already in place, as in Germany, since investment costs can be avoided. Because of that, the study investigates the levelized cost of SNG and hydrogen generation in Germany applying the cost estimation method by Rubin et al. For the investigation, different water electrolysis technologies (alkaline electrolysis, polymer exchange membrane, and solid oxide electrolyzer cell with a size of 1 and 100 MW) and energy scenarios (8,000 h grid, 2,000 h grid, wind, and solar) are contemplated. Besides that, the environmental costs of SNG and hydrogen generation in Germany are investigated due to the increasing importance of these costs for society and companies. The author concludes that the levelized costs of SNG and hydrogen are far too high compared to peer studies, as more cost factors have been considered after applying the method by Rubin et al. In terms of the environmental costs, the use of Germany's grid electricity is not recommended for SNG and hydrogen generation since

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Abbreviations

AACE	Association for the advancement of cost engineering
AEL	Alkaline-Electrolysis
BEC	Bare Erected cost
CAPEX	Capital expenditure
CF	Capacity factor
ct	Cent
DAC	Direct-Air-Capture
EPC	Engineering, Procurement, Construction cost
EPRI	Electric Power Research Institute
ESG	Environmental, Social, Governance
FCHO	Fuel Cell and Hydrogen Observatory
FOAK	First of a kind
FOM	Flexible Operating&Maintenance cost
GJ	Gigajoule
Gt	Gigatons
GWP	Global Warming Potential
h	Hour
IEA	International Energy Agency
IEAGHG	International Energy Agency Greenhouse Gas R&D Programme
ILCD	International Life Cycle Data
IPCC	Intergovernmental Panel on Climate Change
kg	Kilogram
KOH	Potassium hydroxide
kW	Kilowatt
kWh	Kilowatt hour
LC	Levelized Costs
LCA	Life-Cycle-Assessment
LCOE	Levelized cost of electricity
LHV	Lower Heating Value
MEA	Monoethanolamine
MW	Megawatt
MWh	Megawatt hour
NaOH	Sodium hydroxide
NETL	National Energy Technology Laboratory
NG	Natural gas
OEM	Original Equipment Manufacturer

OPEX	Operating expenses
PEM	Polymer-Exchange-Membrane
PtH	Power-to-Hydrogen
PtM	Power-to-Methane
PV	Photovoltaik
ReCiPe	Method of calculating environmental impacts
SI	Supplementary Information
SNG	Synthetic Natural Gas
SOEC	Solid-Oxide-Electrolyzer-Cell
TASC	Total As-Spent Cost
TOC	Total Overnight Cost
TPC	Total plant cost
USD, \$	US-Dollar
VAT	Value-Added Taxes
VOM	Variable Operating&Maintenance cost
WACC	Weightes Average Cost of Capital

miscellaneous

CH ₄	Methane
CO ₂	Carbon dioxide
H ₂ S	Hydrogen sulphide
O ₂	Oxygen
m ³	Cubic meter
Nm ³	Standard cubic metre
°C	Degrees Celsius
€	Euro

units

CO ₂ -eq	Carbon dioxide equivalent
CFC-eq	Trichlorofluoromethane equivalent
1.4 db-eq	1.4 dichlorobenzene equivalent
PM _{2.5} -eq	Particulate Matter less than 2.5-µm equivalent
kBq U ²³⁵ -eq	Kilobecquerel of Uranium-235 equivalent
NM VOC-eq	Non-Methane Volatile Organic Compounds equivalents
SO ₂ -eq	Sulphur dioxide equivalent
P-eq	Phosphor equivalent
CTUh	Comparative Toxic Unit for humans
Mol H ⁺ -eq	The molar concentration of hydrogen ion equivalent

Introduction

Due to advancing global warming and the resulting danger for societies, 195 countries signed the Paris agreement in 2015 to mitigate this effect [1]. The agreement's main goal is to limit the temperature increase to 1.5 °C compared to the pre-industrial level by the end of the 21. century. However, the 1.5 °C goal might be reached much earlier if the situation does not change,

and the release of emissions continuous on the same level, as forecasted by the Intergovernmental Panel on Climate Change (IPCC) [1]. In this regard, the IPCC emphasizes the importance of the reduction of CO₂ emissions to net zero by 2050. This means that the same amount of CO₂ released per year needs to be removed from the atmosphere. According to the International Energy Agency (IEA), the amount of CO₂ released in 2020 corresponded to 33.9 Gt CO₂ [2,3]. To achieve this ambitious goal by 2050, nothing less than a fundamental transformation

of the global energy system is necessary. For this, various options are available, e.g., the replacement of fossil power plants by renewables, mostly wind and solar power, and energy efficient retrofits to reduce CO₂ emissions in the field of electricity and heating, the biggest contributor to the overall CO₂ emissions [2]. However, new challenges will occur with regard to the system's transformation, as wind and solar power are not always accessible. In this regard, the generation of synthetic natural gas (SNG), where captured CO₂ and hydrogen are converted into SNG through methanation, and green hydrogen might play an important role in the future to help mitigate this challenge when wind and solar power are not accessible. Because of that, the levelized costs of SNG and hydrogen are of significant interest. In this regard, many studies have already been published on this topic [4–9]. However, there is no study that has considered the method of Rubin et al. [10] and all three major water electrolysis technologies to calculate the levelized cost of SNG and hydrogen. Therefore, this study provides a new perspective on the levelized cost of SNG and hydrogen using this method. In addition, the data and results obtained can be used for future research, highlighting the value of this study to the scientific community. Therefore, this study provides both a new perspective on the levelized costs of SNG and hydrogen and, with the data obtained, a basis for future research work.

Furthermore, the study aims to investigate the environmental costs of SNG and hydrogen generation, which, as reported by Ref. [11], can be viewed as a decline of economic welfare and, therefore, be interpreted as damage costs to society caused by environmental impacts [12,13]. The reason for considering environmental costs is that the fulfilment of environmental standards by companies, such as the Environmental, Social, and Governance (ESG) criteria, is becoming increasingly important and, viewing the future and a net zero emission society, is gaining further significance [14]. For this reason, it is important for companies to know, for example, how much CO₂ emissions are caused by the manufacture of a product and what societal damage costs result. In this way, targeted measures can be taken to reduce emissions and environmental costs, with corresponding benefits for people and nature. Besides that, the awareness of environmental problems and costs has increased in society, as reported by Refs. [15,16]. As environmental costs are normally disregarded in a classical cost study, the consideration of those adds value to this study and its readers.

The next paragraph briefly describes SNG and hydrogen production, whereas reference is made to further literature that describes the processes in more detail.

Hydrogen production

More than 95% of the worldwide produced hydrogen is generated by steam reforming [17], where methane (CH₄) from natural gas is converted into carbon monoxide and hydrogen [18], because the process causes costs of merely 0.045–0.06 €/kWh_{LHV} (Lower-Heating Value) [19]. The costs, however, increased to more than 0.18 €/kWh_{LHV} and thus tripled due to the abnormal rise of natural gas prices in 2022 as a consequence of Russia invading the Ukraine) [20]. Nevertheless, the process is environmentally unfriendly and emits 13.3 kg CO₂/kg H₂ [21]. Consequently, more environmentally friendly options, such as alkaline electrolysis, polymer membrane electrolysis, and solid oxide electrolysis, are essential towards a net zero CO₂ energy system in 2050 since these technologies cause fewer environmental impacts than steam reforming, presupposed, the electricity stems from renewables, as wind and solar energy (see section 3). The heart of the electrolysis technology is the stack, where H₂O is split into its components H₂ and O₂. While H₂ is formed at the negatively charged cathode, O₂ is formed at the positively charged anode [22]. Since the stacks' lifetime is limited, they need to be replaced after a certain period. The lifetime varies between the technologies as shown in Table 1, the same applies to the specific system energy consumption, current density, stack materials, etc (see Table 1). Schiebahn et al. describe the technologies and the production process comprehensively [23].

Nowadays, only around 4% of the world's hydrogen is produced by these three technologies due to the high energy consumption and costs [4]. Hence, the share of green hydrogen is little and requires more support. When it comes to green hydrogen generation, the site selection is of importance. Because of that, renewable Power-to-Hydrogen plants should be situated in coastal areas with a high duration of sunshine, as in these areas a significant amount of renewable electricity can be generated and used to produce hydrogen, for example, in countries like South Africa and South Australia (South Africa aims for one of the lowest green hydrogen generation costs worldwide by 2030) [25,26]. In Germany, the northern parts in Lower Saxony and Sleswick-Holsatia are appropriate for green hydrogen production, according to electricity and natural gas grid operator, as large wind farms are already installed. Then, the produced green hydrogen can be stored in the already existing natural gas grid and can be further supplied to the chemistry and steel industry plants. A generation of green hydrogen close to the chemistry and steel

Table 1 – Comparison of hydrogen technologies [24].

	AEL	PEM	SOEC
Lifetime stack (h)	60,000–90,000	20,000–60,000	<10,000
Cathode material	Ni, Ni–Mo alloys	Pt, Pt–Pd	Ni/YSZ
Anode material	Ni, Ni–Co alloys	IrO ₂	LSM/YSZ
System energy consumption (kWh/m ³ H ₂)	4.5–6.6	4.2–6.6	>3.7
Current density (A/cm ²)	0.2–0.4	0.6–2.0	0.3–2.0
Operating temperature (°C)	60–80	50–80	650–1000
Cell Voltage (V)	1.8–2.4	1.8–2.2	0.7–1.5
Ni (nickel), Mo (molybdenum), Co (cobalt), Pt (platinum), Pd (palladium), IrO (iridium oxide), YSZ (yttria stabilised zirconia, LSM (lanthanum strontium manganite)).			

plants is also theoretically possible. However, an expansion of the electricity grid is necessary for this to transport the green electricity from the coastal areas to the plants, which is difficult and costly, while the supply through the already existing natural gas grid saves costs [27].

Synthetic natural gas production

To produce synthetic natural gas, hydrogen is further processed with CO₂ to SNG through methanation. The reaction happens via the Sabatier process at temperatures between 250 and 400 °C and pressures of 1–80 bar, using nickel as a catalyst. The required CO₂ can be obtained from various sources, as air, industrial processes, power plants, and biomass. In this study, the CO₂ is obtained from air, biomass (grass silage), and a cement plant (flue gas). With regard to the CO₂ capture from the air, the CO₂ is bound with the help of a chemical substance (e.g., NaOH or KOH). The CO₂ is then separated from the substance by adding heat. Afterwards, the CO₂ can be fed into the methanation reactor under pressure [23,28]. In terms of biomass as CO₂ source, the CO₂ containing biogas is produced by fermentation. The fermentation process happens through bacteria. After the fermentation process, the biogas is purified from components such as H₂S, compressed and fed directly into the methanation reactor [23,29]. Regarding the extraction of CO₂ from the flue gas stream of a cement plant, the CO₂ contained in the flue gas stream is absorbed by chemical absorption. For this purpose, a chemical solution of monoethanolamine and water is sprayed onto the flue gas stream from above. The CO₂ is then separated from the amine solution by steam. In a further process step, the CO₂ is also separated from the steam, which is done in a condenser, and fed into the methanation reactor [27]. Because PtM plants are not yet state of the art, cost studies are sparse [23]. More comprehensive information about the process can be received from Schiebahn et al. [23].

Methodology

In this section the cost estimation method after Rubin et al. [10] is explained in detail. This method consists of three different parts: Total As-Spent Capital costs (TASC), fixed & variable Operating & Maintenance costs. Those are introduced in this section besides TASC and scaling factors as well as the equation for the LC calculation. Besides that, the environmental prices for the environmental cost calculation are introduced, as well as the applied energy scenarios.

No specific plants have been considered for the calculation of the LC, as this is a simple cost study intended to provide a new perspective on the LC of SNG and hydrogen, considering the method by Rubin et al. The reason for considering 1 and 100 MW plants is that the data availability for 1 MW plants is very good compared to 100 MW plants. However, generation will most likely occur at large centralized facilities [30]. Therefore, both values for 1 and 100 MW plants have been considered.

Since this study is focused on providing a new perspective on the LC of SNG and hydrogen and offering data for future research, only current data and scenarios have been contemplated (8,000 h grid, 2,000 h grid, wind, and solar).

Scenarios with surplus renewable energy have deliberately not been contemplated, as only about 0.5% of the power generation in Germany can be classified as surplus energy [31], which amounts to approx. 43 h per year [31]. The 2,000 h represent a realistic assumption for the availability of wind (onshore) and solar power in Germany, based on [32,33].

Cost estimation after Rubin et al

The plants' cost estimation is based on Rubin et al. [10] and recommendations of the technical assessment guide by the Electric Power Research Institute (EPRI) [34] as well as the National Energy Technology Laboratory's (NETL) guideline for cost estimations of power plants [35]. The method was originally created for fossil energy systems, but it can also be used for various revenue generating plants, such as PtM and PtH plants [35]. According to Rubin et al. [10], the Bare Erected Cost (BEC) are the crucial element of a cost estimate and consist of process equipment cost, supporting facilities, and direct and indirect labor costs. While the Total Plant Cost (TPC) further include Engineering, Procurement, and Construction cost (EPC) (as well as process and project contingencies), the net Total Overnight Cost (TOC) comprises of additional Owner's Cost, such as preproduction costs, inventory capital, and land. The reasons for considering process and project contingencies come a long with uncertainties related to the technology's advance, and the detailed design of a project. The less developed a technology and a project design are, the higher the process and project contingencies [10]. Since the original equipment manufacturers' (OEM) quotes refer to net prices, a value added tax (VAT) has been added to compute the total TOC. In addition, interests and cost escalations during construction come on top of the total TOC, thus receiving the TASC [35]. Because this cost study is a class 4 cost estimate, in line with the Advancement of Cost Engineering International (AAACE), an accuracy rate of ±30% is taken into account [36].

Table 2 gives an overview of the methodology. The generated data stem either from OEMs, literature, or estimations. Moreover, the calculations of the plants' TASC can be found in the Supplementary Information (SI) section 1, including detailed information for the reader's understanding.

Besides the TASC costs, the operating expenditures (OPEX) are essential to compute the LC. According to Rubin et al. [10], the OPEX can be subdivided in two categories. The fixed OPEX (FOM, fixed Operating & Maintenance cost) and the variable OPEX (VOM, variable Operating & Maintenance cost). While the FOM include cost that occur even if the plant is not operating, as labor costs, administrative and support labor, maintenance materials, and insurances, the VOM comprises of costs that emerge only if the plant is operating, such as electricity and water costs. The cost items of FOM and VOM are listed in Table 3, following Rubin et al. [10]. Note that the terms fixed OPEX and FOM as well as variable OPEX and VOM can be used similarly in this study.

TASC factor

The TASC factor is the ratio between the Total As-Spent Capital cost and the Total Overnight Cost and expresses the additional cost on top of the TOC due to interest and

Table 2 – Calculation of Total As-Spent Capital cost [10,34,35].

Cost items	Sum of the cost elements	Comments
Process equipment cost		Total net process equipment cost
+Supporting facilities		10% of process equipment cost
+Labor cost (direct and indirect)		Based on constructor's information
	= Bare Erected Cost (BEC)	
+Engineering service cost		15% of BEC
	= Engineering, Procurement, Construction cost (EPC)	
+Process contingency		40% of BEC
+Project contingency		30% of the sum of BEC, EPC fees and process contingency
	= Total Plant Cost (TPC)	
+Owner's cost		
Preproduction (Start-up) costs		2% of TPC
Inventory capital		0.5% TPC
Land		100 €/m ²
Financing cost		2.7% of TPC
Other Owner's cost		15% of TPC
	= Net Total Overnight Cost (TOC)	
+Value added tax VAT		19% of net TOC
	= total TOC	
+Interest and cost escalation during construction		TOC times TASC factor
	= Total As-Spent Capital (TASC)	
	±30% Accuracy rate	According to AACE Class 4 estimate

Note that the terms TASC and capital expenditure (CAPEX) can be used similarly in this study.

escalation expenses during the construction phase [35]. To calculate the TASC factor, the following assumptions are made (see Table 4). The financial structure of the investor-owned utility is 55% debt and 45% equity. The debt's interest is assumed to be as high as 10%, based on expert judgement [42], the same value as the return on equity, following historical data of the Standard & Poor's 500 Index [43]. Thus, the Weighted Average Cost of Capital (WACC) yields 10%.

Subsequently, the following calculations with an escalation rate of 3% (nominal) and a WACC of 10% have been conducted to calculate the TASC factors using Eq. 1-3 [35]. The capital expenditure (construction) period for 1 MW PtM and

PtH plants is 1 year, whereas the capital expenditure period for 100 MW PtM and PtH plants is 3 and 2 years, respectively. The calculated TASC factors are shown in Table 5.

$$\frac{TASC}{TOC} = Escalation + cost\ of\ funding \quad Eq.1$$

$$Escalation = \sum_{n=1}^y [(1+i)^{(n-1)} * \%Capital\ expenditure_n] \quad Eq.2$$

$$Cost\ of\ Funding = \sum_{n=1}^y WACC * (y - n + 1) * (1+i)^{(n-1)} * \%Capital\ expenditure_n \quad Eq.3$$

With:

Table 3 – Calculation of fixed and variable Operating & Maintenance cost [10,34,35,37].

Cost items	Sum of the cost elements	Comments
Operating labor		Based on expert judgement
Maintenance labor		2% of TPC, of which 40% are assigned to maintenance labor (default estimate by EPRI and IEAGHG [10])
Administrative and support labor		30% of O&M labor (sum of the above)
Maintenance materials		2% of TPC, of which 60% are assigned to maintenance materials (default estimate by EPRI and IEAGHG [10])
Insurance		2% of TPC
	= FOM costs	
Consumables		
Electricity		Price of 16.94 ct/kWh (grid), 6 ct/kWh (wind), and 7 ct/kWh (solar) [38,39]
Water		Price of 0.00212 €/l [40]
CO ₂ costs (grass silage)		For PtM with biomass as the CO ₂ source, assuming a price of 30 €/t [41]
	= VOM costs	

Note that the author used the electricity prices (grid) for industry costumers in Germany, as the production of hydrogen and SNG is energy intensive. Compared to the electricity prices for the private sector, these prices are considerably lower. The prices are based on the values for 2021, as no current values were available. They can be found here [38]. For wind and solar power sources, the author considered cost data in ct/kWh released by Fraunhofer [39]. For water, the author considered the average price for tap water in the region (Lower Saxony), knowing that the prices can differ significantly between different places [40]. These values are valid as they have been published by trustworthy organisations/institutions such as the ministry of economics in Lower Saxony, Statista Company, and Fraunhofer Research Institute.

Table 4 – Financial structure of investor-owned utility.

Type of Security	Share in %	Current Euro costs	Weighted Average Cost of Capital
Debt	55%	10%	5.5%
Equity	45%	10%	4.5%
Total	100%	20%	10%

n = The year of capital expenditure
 y = Total number of years of capital expenditure
 i = escalation rate (3%)
 %Capital expenditure_n = % of Capital expenditure in year n
 WACC = Weighted average cost of capital.

Scaling factor

In order to scale the costs from 1 to 100 MW plants, the equation below (Eq. 4) is employed, according to Remer and Chai [44]. With regard to the process equipment costs, a scaling factor of 0.88 is applied for the stacks, while a factor of 0.7 is assumed for the remaining equipment [45,46]. The scaling factors for the stacks have been chosen following [45], as they have done a comprehensive study on the economies of scale of power-to-gas systems. They applied a scaling factor of 0.88 for AEL stacks, 0.89 for PEM stacks, and 0.87 for SOEC stacks. The author decided to use an average of 0.88 for the stacks to simplify the process, as the values do not deviate a lot. Besides that, they have also calculated scaling factors for the other parts of the systems. As the values are in the range of 0.7 [45], the author decided to use this value as this factor is an average factor that is usually used in cost scaling and simplifies the calculation process, following Zhang et al. [46].

$$\frac{c_2}{c_1} = \left(\frac{x_2}{x_1}\right)^b \tag{Eq.4}$$

c₁ = Cost of component
 c₂ = Unknown value
 x₁ = Size of plant 1 (1 MW)

x₂ = Size of plant 2 (100 MW)
 b = Scaling factor 0.7 or 0.88

Levelized cost of SNG and hydrogen

In order to calculate the profitability of a plant, there are various methods [47,48]. One of the methods is the net present value, which provides information on whether it is worth investing in a project/plant or not. This involves subtracting the total discounted costs (capital and operating costs) from the total discounted revenues over the lifetime of a project. A positive result means it is worth investing in the plant or project [47,48]. Another method is to calculate the levelized cost of electricity (LCOE) or in terms of SNG and hydrogen production the levelized cost of synthetic natural gas or hydrogen. According to Fambri et al., the breakeven sale price is calculated with this method, which means that this value must be achieved at least in order to avoid losses [49]. This value is expressed in cost per unit of stored energy (e.g. €/kWh or €/MWh). The calculation of the levelized cost in this study is based on Rubin et al., using the following equation.

$$LC = \frac{\sum_{t=1}^n (CAPEX_t + FOM_t + VOM_t) * (1 + r)^{-t}}{\sum_{t=1}^n (electricity\ generated_t) * (1 + r)^{-t}} \tag{Eq.5}$$

CAPEX_t = Capital expenditure during construction in year t.
 FOM_t = Fixed Operating & Maintenance cost in year t.
 VOM_t = Variable Operating & Maintenance cost in year t
 r = Discount rate.
 Electricity generated_t = Electricity generated in year t
 n = Lifetime of plant.

Note that costs for decommissioning are not included, assuming that these costs will be covered by the plants' salvage value, as reported by Ref. [50]. Moreover, the discount rate and WACC are the same (10%), as many companies use

Table 5 – Overview of TASC factors.

1-year TASC/TOC, nominal H ₂ and SNG (1 MW)					
Cost year	Escalated cost	Cost of funding	WACC	Escalation	Capital expenditure
2021	1.00	0.10	10%	0%	100%
Total	1.000000	0.100000			
TASC/TOC	1.100000				
2-year TASC/TOC, nominal H ₂ 100 MW					
2021	0.400000	0.04000	10.00%	0%	40%
2022	0.618000	0.10300	10.00%	3%	60%
Total	1.018000	0.143000			
TASC/TOC	1.161000				
3-year TASC/TOC, nominal SNG 100 MW					
2021	0.10	0.010	10.00%	0%	10%
2022	0.52	0.062	10.00%	3%	50%
2023	0.42	0.106	10.00%	3%	40%
Total	1.04	0.178			
TASC/TOC	1.21725				

the WACC as the discount rate when calculating and budgeting for a new project [51].

Overview of basic details

After discussing essential assumptions and information of the cost estimate, Table 6 gives a short overview of basic details.

Environmental costs

The environmental costs are calculated based on environmental prices at midpoint level published by CE Delft [13]. Table 7 shows the prices for each impact category that is considered in the study. Since the environmental prices by CE Delft have been created based upon ReCiPe, some differences compared to the ILCD midpoint method (applied for the calculations of environmental impacts) occur. However, these differences have not been further investigated because both ReCiPe and ILCD use identical techniques and literature on many themes [13]. Hence, the same environmental prices as for ReCiPe have been assumed to be suitable for calculating the environmental costs, using results generated by the ILCD method. Although, the values for human toxicity and acidification have been adjusted since the metrics between both methods deviate. Subsequently, the ILCD results for human toxicity and acidification have been converted with a factor of 5,540,208 kg 1.4 db-eq./CTUh and 1.37 SO₂-eq./mol H⁺-eq.,

respectively [52]. This is a common practice in agreement with [53]. Moreover, the prices refer to 2015 and do not change, as assumed by the handbook's authors (conservative approach), except for climate change [13]. This value increases by 3.5% per year (see Table 7) [13]. Note that the values for climate change have been generated using IPCC 2013, GWP 100a, and the prices refer to 2019 because no recent data for the energy scenario (see next paragraph) were available at that start of modelling.

Energy scenarios

The energy scenarios (grid, wind, and solar) that have been used to compute the environmental impacts of SNG and hydrogen production are demonstrated in Fig. 1. For the grid scenario, Germany's energy scenario in 2019 has been chosen [54]. Although, the energy production from oil (0.4%) could not be depicted due to missing availability in the software's database. The computation has been done utilising the Umberto LCA + software, version 3.5. The software makes it possible to estimate the potential environmental impacts of a product. Predefined processes from the database are used for this purpose. Based on these processes, the software can calculate the potential environmental impacts after all energy and mass data have been entered. Subsequently, the results have been multiplied with the environmental prices in Table 7 to calculate the environmental costs. The results stem from

Table 6 – Overview of basic details.

Type of plant	First-of-a-kind (FOAK)
Year and currency of cost estimate	2021, Euro (€), current Euro values (nominal)
Interest and escalation during construction	10%, 3%
Inflation rate materials, insurance, VOM	3%,
Escalation rate labor	2.5%
Capital expenditure period	1 MW PtH and PtM plants: 1 year 100 MW PtH plants: 2 years 100 MW PtM plants: 3 years
Operational Period	20 years
Economic Analysis Period	21, 22, and 23 years (sum of capital expenditure period and operational period)
Distribution of capital expenditure	1 year: 100%, 2 years: 40%, 60%, 3 years: 10%, 50%, 40%
Weighted average cost of capital	10%
Discount rate	10%

Table 7 – Environmental prices [13].

Impact category	unit ReCiPe	unit ILCD/IPCC	2015	2019
Climate change	€/kg CO ₂ -eq.	€/kg CO ₂ -eq.	0.0566	0.0649
Ozone layer depletion	€/kg CFC-eq.	€/kg CFC-eq.	30.4	30.4
Human toxicity	€/kg 1.4 db-eq.	CTUh	0.0991	0.0991
Particulate matter formation	€/kg PM _{2.5} -eq.	€/kg PM _{2.5} -eq.	39.2	39.2
Ionizing radiation	€/kg kBq U ²³⁵ -eq.	€/kg kBq U ²³⁵ -eq.	0.0461	0.0461
Photochemical oxidant formation	€/kg NMVOC-eq.	€/kg NMVOC-eq.	1.15	1.15
Acidification	€/kg SO ₂ -eq.	mol H ⁺ -eq.	4.97	4.97
Freshwater eutrophication	€/kg P-eq.	€/kg P-eq.	1.86	1.86

previous studies published by the author [55,56] and are shown in the SI section 4, together with the calculated environmental costs.

Results and discussion

The levelized and environmental costs of SNG and hydrogen generation in Germany are discussed in this section. In order to make the discussion more manageable, the results are

listed in figures and tables. Moreover, the CAPEX calculation can be found in the SI section 1.

As shown in Fig. 2, the CAPEX of 1 MW PtH plants range from about 8800 to 11,400 €/kW. In contrast, the CAPEX of the 100 MW PtH plants, assuming a two-year construction phase, are between about 4100 and 6000 €/kW, which is approx. 50% lower (see Fig. 3). The lesser costs emerge due to scaling effects, considering the scaling factors described in section 2, as a linear cost increase from 1 to 100 MW is not assumed, which is in line with [6]. The same is valid for

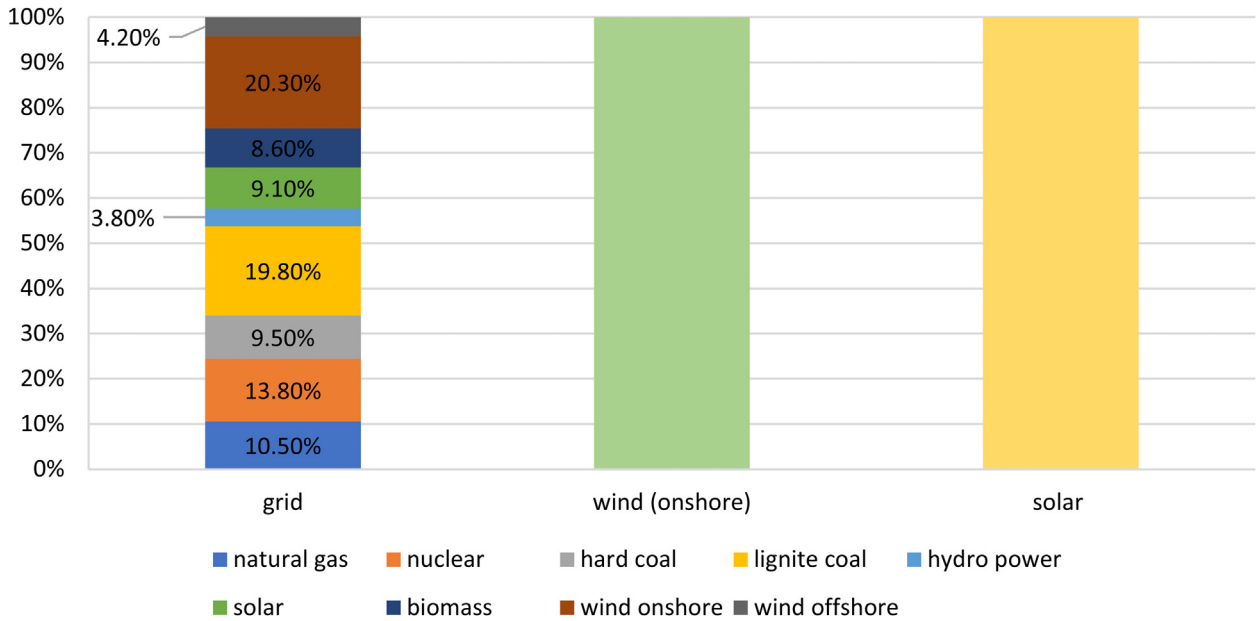


Fig. 1 – Overview of energy scenarios.

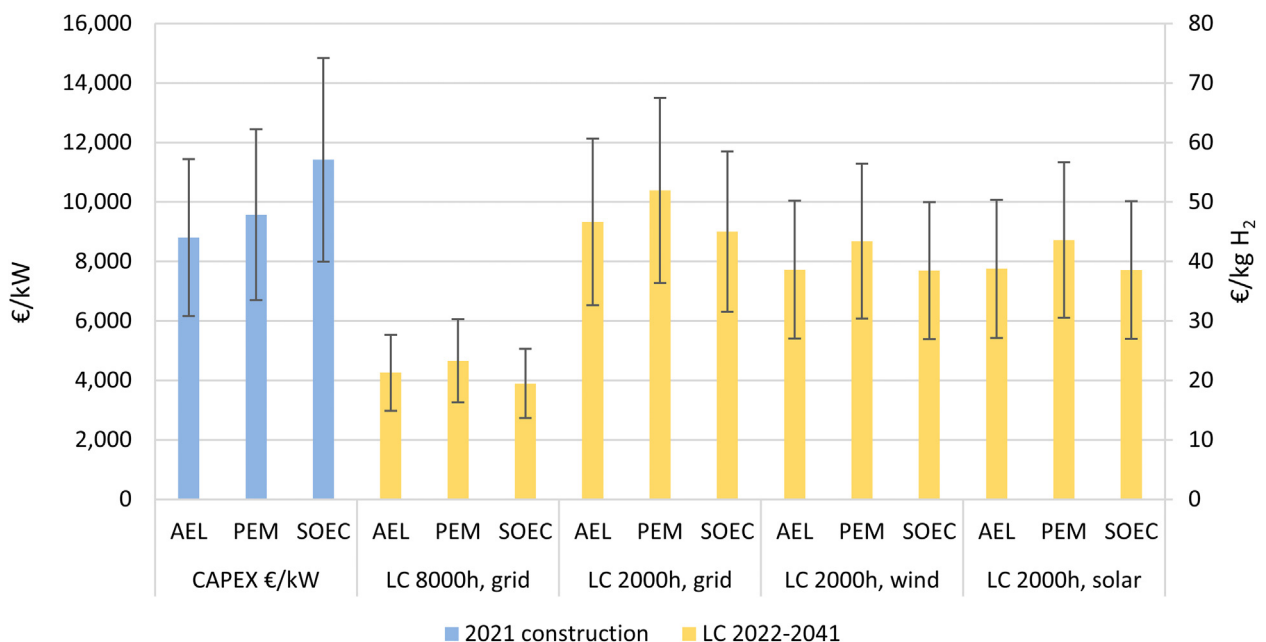


Fig. 2 – CAPEX and LC of H2 in 1 MW PtH plants.

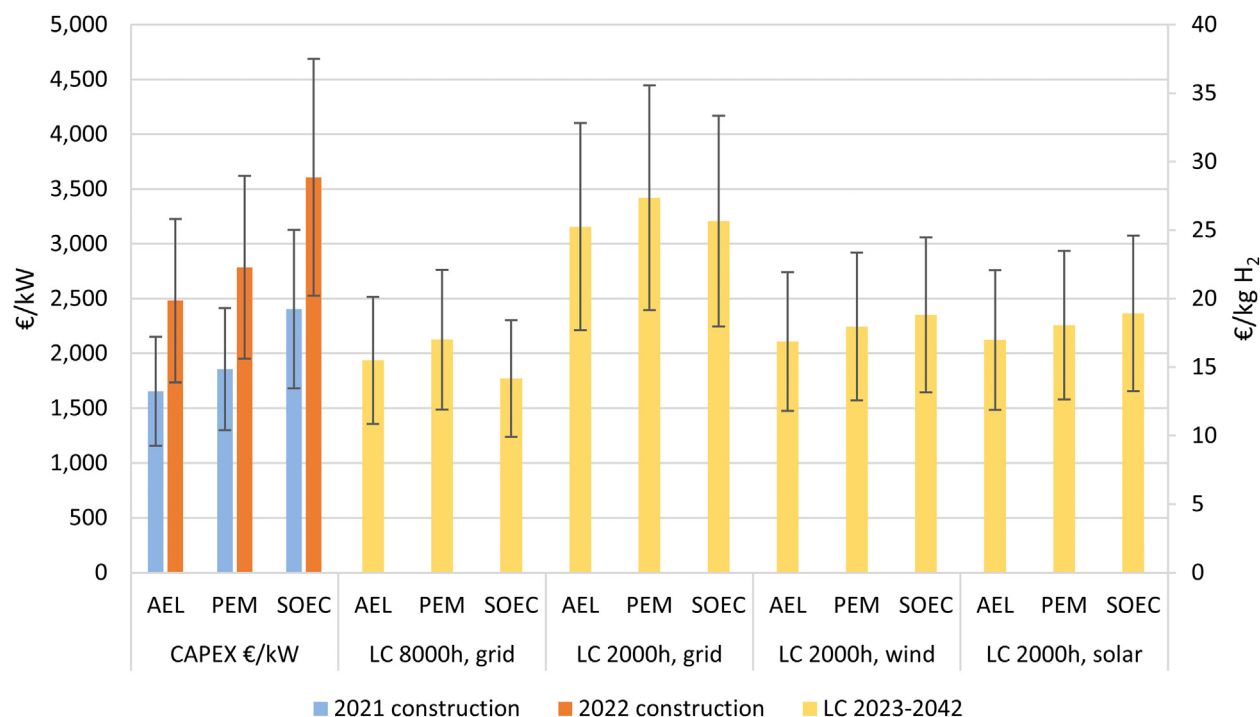


Fig. 3 – CAPEX and LC of H₂ in 100 MW PtH plants.

the LC of hydrogen, which for the 100 MW plants are about 27% (8,000 h, grid), 45% (2000h, grid) and 50–58% (2,000 h, wind/solar) lower and range in between 14 and 17 €/kg H₂ (8,000 h, grid), 25.2–27.3 €/kg H₂ (2,000 h, grid) and 16.9–19 €/kg H₂ (2,000 h, wind/solar), without accuracy range (see Fig. 3).

Besides that, the LC of hydrogen (wind and solar, 2000h) are nearly the same (see Figs. 2–3). The reason is that only the electricity price for wind and solar is different (see Table 3), while the other costs are identical.

The same applies to the CAPEX and LC of SNG in 1 and 100 MW PtM plants (see Figs. 1–2 in the SI and Tables 8–10). The CAPEX for the 1 MW PtM plants are in between 14,710 and 35,075 €/kW, while the CAPEX for the 100 MW plants are in between 5977 and 12,875 €/kW and thus around 60% lower compared to the CAPEX of 1 MW plants. Moreover, the LC of SNG in the 8000 h grid scenario for PtM plants with DAC lie in the range of 10.46–12.21 €/kg SNG, while the results for plants with biomass and cement as the CO₂ source are in between

4.10 and 4.80 €/kg SNG and 8.37–9.93 €/kg SNG, respectively. These values are approx. 50% (DAC), 38% (biomass), and 35% (cement) lower than the values for 1 MW plants. For the 2000h scenarios, these values lie in between 20.82 and 25.67 €/kg SNG (DAC, grid), 7.97–8.87 €/kg SNG (biomass, grid), 16.39–18.25 €/kg SNG (cement, grid), and 16.21–20.79 €/kg SNG (DAC, wind), 6.12–6.84 €/kg SNG (biomass, wind), 11.93–13.47 €/kg SNG (cement, wind), respectively, 16.25–20.84 €/kg SNG (DAC, solar), 6.13–6.86 €/kg SNG (biomass, solar), 11.97–13.51 €/kg SNG (cement, solar). These values are 50–65% (2000h, grid), 57–71% (2000h, wind), and 57–70% (2000h, solar) lower than the values for 1 MW plants. The graphical illustration of CAPEX and LC of SNG for 1 and 100 MW PtM plants can be found in the SI section 5.

The reason for the lower values of PtM plants with biomass as the CO₂ source compared to PtM plants with air and cement as the CO₂ source is due to the fact that the contained methane in the biogas (assumed share of 53%, see SI section 3) is also classified as SNG, resulting in higher production volumes that

Table 8 – CAPEX of 1 MW and 100 MW PtM plants.

PtM plant type	CAPEX 1 MW plant in €/kW (1 year)	CAPEX 100 MW plant in €/kW (3 years)	Reduction of costs
PtM-AEL-DAC	29,602	10,116	66%
PtM-PEM-DAC	29,844	10,502	65%
PtM-SOEC-DAC	35,075	12,875	63%
PtM-AEL-Biogas	18,615	6,887	63%
PtM-PEM-Biogas	18,980	7,352	61%
PtM-SOEC-Biogas	21,926	9,090	59%
PtM-AEL-Cement	14,710	5,977	59%
PtM-PEM-Cement	15,371	6,480	58%
PtM-SOEC-Cement	17,934	8,112	55%

Table 9 – LC of SNG in 1 and 100 MW PtM plants applying the 8,000 h and 2,000 h grid scenarios.

PtM plant type	LC in €/kg SNG, 8,000 h grid			LC in €/kg SNG, 2,000 h grid		
	1 MW	100 MW	Reduction	1 MW	100 MW	Reduction
PtM-AEL-DAC	21.55	10.64	51%	59.25	20.82	65%
PtM-PEM-DAC	22.87	12.21	47%	62.96	25.67	59%
PtM-SOEC-DAC	19.83	10.46	47%	55.65	23.17	58%
PtM-AEL-Biogas	7.19	4.44	38%	18.09	8.03	56%
PtM-PEM-Biogas	7.67	4.80	37%	19.36	8.87	54%
PtM-SOEC-Biogas	6.52	4.10	37%	16.73	7.97	52%
PtM-AEL-Cement	14.20	9.11	36%	35.06	16.45	53%
PtM-PEM-Cement	15.33	9.93	35%	38.14	18.25	52%
PtM-SOEC-Cement	12.91	8.37	35%	32.91	16.39	50%

Table 10 – LC of SNG in 1 and 100 MW PtM plants applying the 2,000 h wind and solar scenarios.

PtM plant type	LC in €/kg SNG, 2,000 h wind			LC in €/kg SNG, 2,000 h solar		
	1 MW	100 MW	Reduction	1 MW	100 MW	Reduction
PtM-AEL-DAC	55.00	16.21	71%	55.08	16.25	70%
PtM-PEM-DAC	58.46	20.79	64%	58.55	20.84	64%
PtM-SOEC-DAC	52.12	19.35	63%	52.19	19.39	63%
PtM-AEL-Biogas	16.32	6.12	63%	16.36	6.13	62%
PtM-PEM-Biogas	17.50	6.84	61%	17.54	6.86	61%
PtM-SOEC-Biogas	15.28	6.40	58%	15.31	6.41	58%
PtM-AEL-Cement	30.89	11.93	61%	30.97	11.97	61%
PtM-PEM-Cement	33.74	13.47	60%	33.83	13.51	60%
PtM-SOEC-Cement	29.48	12.67	57%	29.54	12.69	57%

significantly reduce the LC. Besides that, the CAPEX and LC of PtM plants with air as CO₂ source are the highest because of the high CAPEX for the CO₂ separation plant, which is around 5000 €/kW for 1 MW PtM plants according to own estimates based on information from the OEM Climeworks [57]. These costs are reduced to approx. 1500 €/kW for 100 MW plants due to scaling effects (see SI section 1).

The LC of SNG and hydrogen can be seen as very high compared to peer studies (see Table 11). The reason is that the method by Rubin et al. considers more cost factors, such as project and project contingencies, than the methods chosen by peers [5–9]. The results are also far higher compared to natural gas prices and steam reforming (see Table 11, and chapter 1.1). Since different methods and assumptions have

Table 11 – Comparison values of peer studies, including natural gas price [4–9,58,59].

Author/Institution	value	Comment	Conversion factor	Value in €/kg SNG/H ₂
Szima/Cormos	43.56 €/Gj	SNG from PV electrolysis, 85 €/MWh	277.78 kWh/Gj + 33.33 kWh/kg _{LHV} [60,61]	5.22 €/kg
Gutierrez/Antón	0.52 €/kg	H ₂ prod. at 0 €/MWh		0.52 €/kg
Gutierrez/Antón	1.90 €/kg	H ₂ prod. at 25 €/MWh		1.90 €/kg
Gutierrez/Antón	0.26 €/Nm ³	SNG prod. at 0 €/MWh	0.668 kg/Nm ³ CH ₄ [45]	0.39 €/kg
Gutierrez/Antón	0.72 €/Nm ³	SNG prod. at 25 €/MWh		1.08 €/kg
Gorre et al.	137.36 €/MWh	SNG 2030 at 25 €/MWh, 2,000 h	13.9 kWh/kg _{LHV} [62]	1.91 €/kg
Gorre et al.	88.85 €/MWh	SNG 2050 at 25 €/MWh, 2,000 h		1.24 €/kg
Gorre et al.	85.12 €/MWh	SNG 2030 at 25 €/MWh, 6,000 h		1.18 €/kg
Gorre et al.	60.95 €/MWh	SNG 2050 at 25 €/MWh, 6,000 h		0.85 €/kg
Zauner et al.	42.8 ct/kWh _{LHV}	SNG 2020, 100% PV, 1,395 h		5.95 €/kg
Zauner et al.	20.8 ct/kWh _{LHV}	SNG 2030, 100% PV, 1,395 h		2.89 €/kg
Zauner et al.	28.5 ct/kWh _{LHV}	SNG 2020, 100% wind, 3,101 h		3.96 €/kg
Zauner et al.	16.7 ct/kWh _{LHV}	SNG 2030, 100% wind, 3,101 h		2.32 €/kg
Zauner et al.	14.6 ct/kWh _{LHV}	SNG 2050, 100% grid, 8,000 h		2.03 €/kg
Blanco et al.	12.5 €/Gj	SNG realistic scenario	See Szima/Cormos	1.5 €/kg
Lazard Limited	2.30–2.45 \$/kg	H ₂ prod. 1 MW AEL, 30 \$/MWh	0.88 €/€ [63]	2.02–2.15 €/kg
Lazard Limited	2.85–2.90 \$/kg	H ₂ prod. 100 MW PEM, 30 \$/MWh		2.5–2.55 €/kg
Lazard Limited	1.55–1.75 \$/kg	H ₂ prod. 1 MW AEL, 30 \$/MWh		1.36–1.54 €/kg
Lazard Limited	1.85–2.15 \$/kg	H ₂ prod. 100 MW PEM, 30 \$/MWh		1.63–1.89 €/kg
FCHO	4.93–7.49 €/kg	H ₂ prod. 100% PV, different CFs		4.93–7.49 €/kg
FCHO	3.51–6.71 €/kg	H ₂ prod. 100% wind, different CFs		3.51–6.71 €/kg
NG price	9.5 ct/kWh	Market price of natural gas (NG)	13.1 kWh/kg [64]	1.24 €/kg

been applied in the studies, a detailed comparison of the results does not add value to the study.

In the next paragraph, the author sheds some light on the environmental costs of SNG and hydrogen generation.

Environmental costs of SNG and hydrogen generation

As already mentioned in the introduction, the environmental costs of products are becoming increasingly important, which is, why the environmental costs of SNG and hydrogen generation are additionally considered in this study. For the calculation of the environmental costs, the environmental impacts for the production of 1 kg SNG and hydrogen in 1 MW plants, which have been taken from two other studies of the author [55,56], have been multiplied with the environmental prices in Table 7 to calculate the environmental costs. Note that the environmental impacts refer only to 1 MW PtM and PtH plants because no relevant data for 100 MW plants were available.

As can be seen in Fig. 4, the environmental costs of SNG production from grid electricity are many times higher (in some cases by a factor of 10) than the production from wind or solar power. Consequently, the production from grid electricity is not recommended from an environmental perspective, whereas the production from wind power is preferable over solar power. When comparing the technologies, it can be seen that the PtM-SOEC plants cause less environmental costs than the other technologies using grid electricity. This is due to the lower electricity consumption of the technology (see Tab. 15 SI), which leads in particular to lower environmental costs through the impact categories climate change and freshwater & terrestrial acidification, whose main causer are fossil fuels (hard/lignite coal, natural gas) and electricity generation from biogas (biomass), respectively. This effect weakens, however, if the production is from 100% wind or solar power since fossil fuels and biogas are no longer used for electricity generation, so that the results do not differ greatly

even if the electricity consumption of PtM-AEL and PtM-PEM plants are higher.

The same applies to the production of hydrogen (see Fig. 5). The SOEC technology causes less environmental costs when grid electricity is used for hydrogen production due to its lower electricity consumption. The lower environmental costs, as with SNG production, are due to the lower environmental impacts caused by the impact categories climate change and freshwater & terrestrial acidification. In addition, the technologies' environmental costs are almost the same when producing hydrogen from wind or solar power, whereby wind power is preferable over solar power as well.

In Fig. 6, the environmental costs of hydrogen generation are compared to the occurring environmental costs of steam reforming, the most common hydrogen generation process these days [17]. Due to lack of information, only the CO₂ emissions of steam reforming could be considered. For this, a value of 13.3 kg CO₂ per kg H₂ has been contemplated to compute the environmental costs of steam reforming [21]. As shown in Fig. 6, these costs are remarkably higher than the costs caused by the wind and solar scenario (note that only CO₂-eq. have been considered for an equal comparison). Consequently, the hydrogen generation from steam reforming is less attractive from an environmental perspective than the renewable scenarios, especially from the background of increasing CO₂ emissions in the atmosphere and the progressing climate change.

However, the generation costs of hydrogen from steam reforming are lower (1.5–2 €/kg H₂ [19]). Therefore, most hydrogen is produced by steam reforming from fossil fuels due to economic interests, even though the process emits 13.3 kg CO₂ emissions per kg H₂ [21]. Moreover, it must be mentioned that the German government subsidises fossil fuels with more than 16 billion euros per year which might affect those costs [65], but further research needs to be done to show if the government's subsidies affect the hydrogen

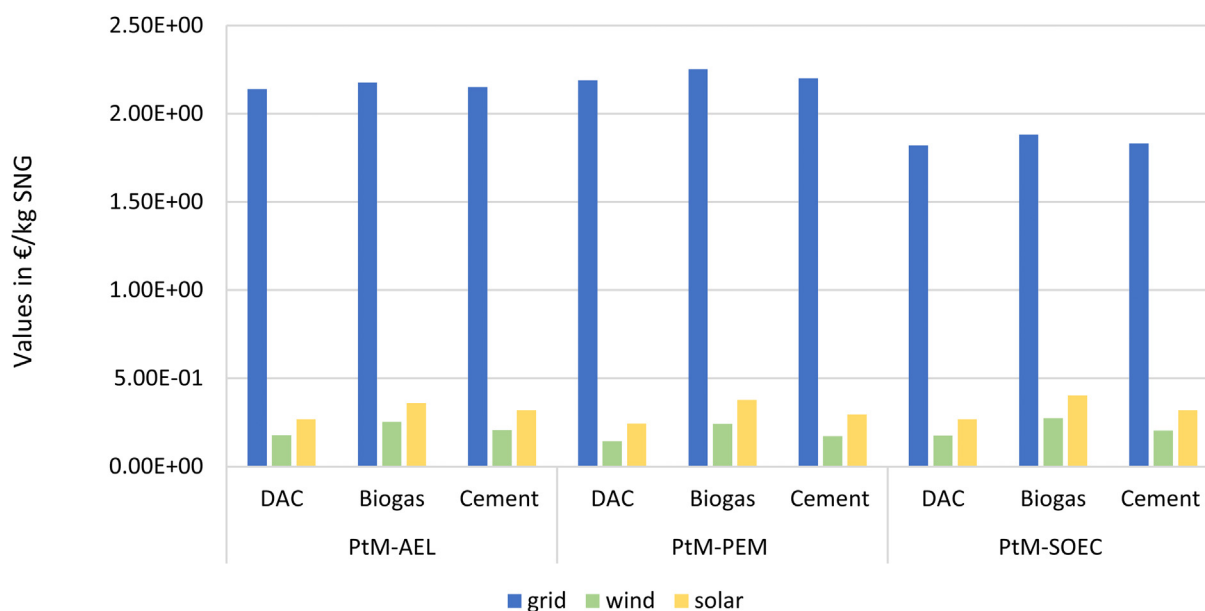


Fig. 4 – Environmental costs of SNG production.

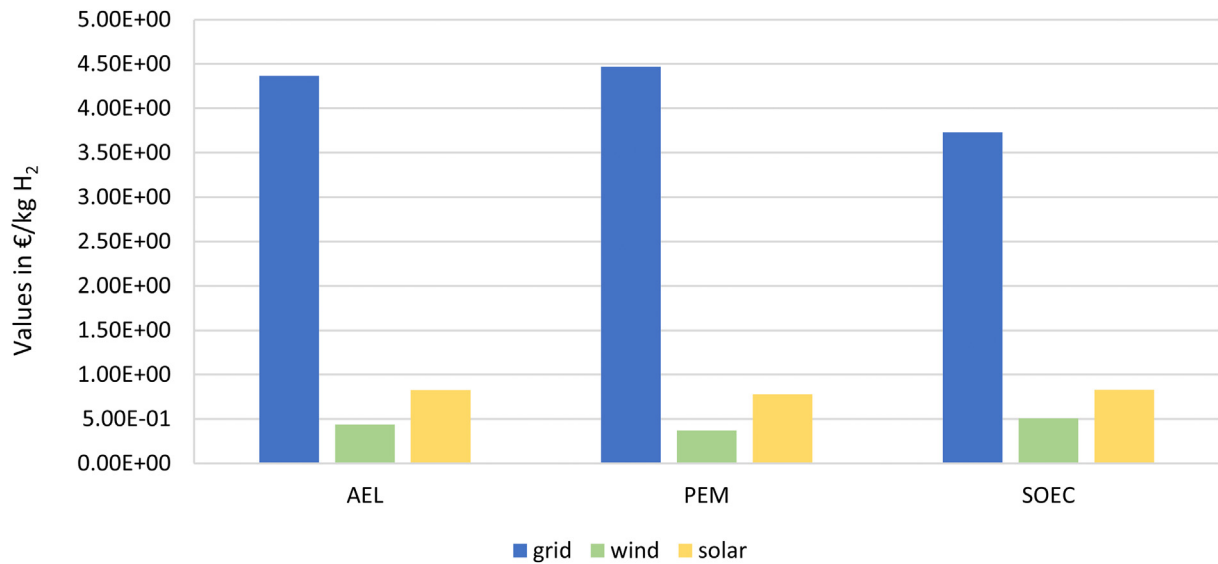


Fig. 5 – Environmental costs of hydrogen production.

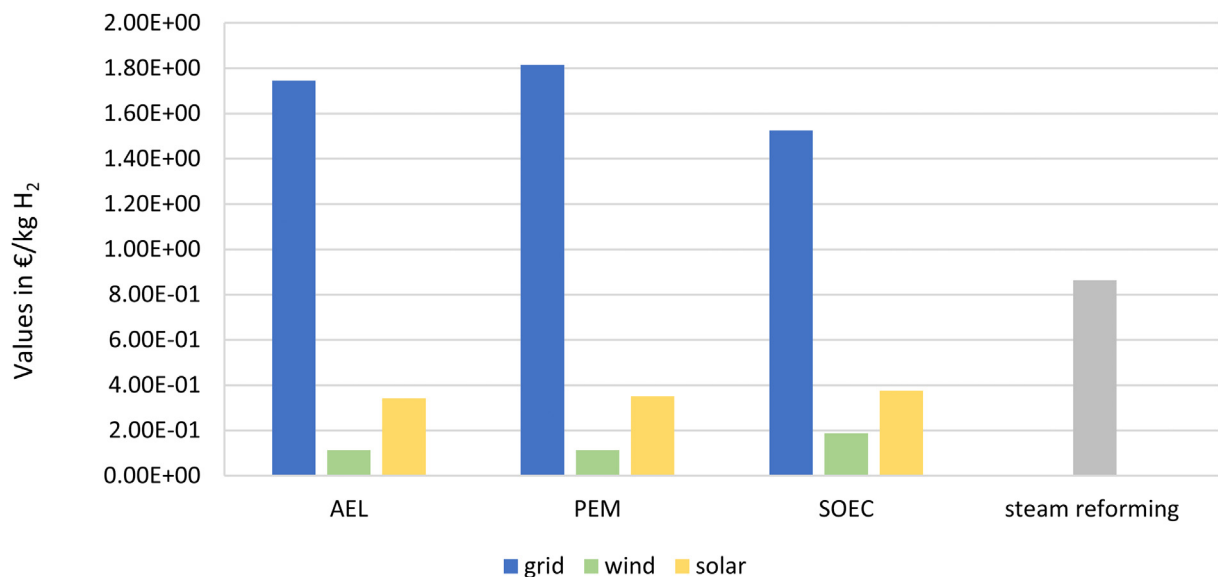


Fig. 6 – Environmental costs of hydrogen production compared to steam reforming (only CO₂/CO₂-eq.).

production by steam reforming. Overall, the results show that SNG and hydrogen production from renewables cause considerably fewer environmental costs and thus damage costs to society than production processes involving fossil fuels.

The LC of SNG and hydrogen are currently far too high compared to natural gas prices (as of mid-Jan 2023 [66]) and steam reforming, as stated above. However, the increase in natural gas prices in 2022 led to an increase of fossil-based hydrogen to more than 6 €/kg H₂ [20]. This means that green hydrogen (in the range of 2.8–6 €/kg) is already cheaper than fossil-based hydrogen produced by steam reforming, considering the high natural gas prices [67]. Besides that, what can be done to lower the LC of SNG and hydrogen as well as to

increase the costs of fossil-based hydrogen, so that environmental impacts can be reduced? In this regard, financial incentives could be initiated that make investments in these technologies more attractive. For example, investors who invest in sustainable technologies such as PtM and PtH could be rewarded with tax breaks. This could drive technological progress, so that lower costs can be achieved.

In addition, the subsidies for fossil energies, which amount to 16 billion Euros in Germany [65] and are contradictory to climate goals, could be invested in reducing the electricity costs, which are a main component of the LC. Consequently, for example, if the electricity price for the 8,000 h scenario is reduced by 50% from approx. 17 ct/kWh to 8.5 ct/kWh, the LC can be reduced by approx. 16% (for 1 MW PtM plants), 28% (for

100 MW PtM plants), 25% (1 MW PtH plants) and 34% (for 100 MW PtH plants). Based on the 8,000 h scenario of the 100 MW PtH plants, this would mean that the costs can be reduced from about 14 to 16.8 €/kg H₂ to about 9.33–11.2 €/kg H₂, which corresponds to about 28–33.6 ct/kWh_{LHV} at a lower heating value of 33.33 kWh/kg H₂ [61]. Thus, the electricity price has a great leverage effect on the LC and shows that it is a sensitive parameter. This could be a starting point for decision-makers in order to make investments more attractive.

Besides that, fossil processes such as steam reforming which emit far more environmental impacts compared to green processes (see above) could be charged with an environmental tax. The environmental costs (calculated above) could be considered for this. For example, the difference of the environmental costs between a fossil and green process could be used and added to the production costs. Thus, fossil-based hydrogen produced by steam reforming would be more expensive, favoring green hydrogen.

Conclusion

Power-to-Gas technologies are of interest to mitigate challenges that may arise due to the energy system transformation, as wind and solar power are not always accessible. Therefore, the LC of SNG and hydrogen generation in Germany have been investigated in this study, considering the three main water electrolysis technologies and different energy scenarios. For this, the method by Rubin et al. has been used, which has not done before for a cost study that includes all three main water electrolysis technologies to the knowledge of the author. Therefore, this study provides a new perspective on the levelized cost of SNG and hydrogen using this method. In addition, the data and results obtained can be used for future research, highlighting the value of this study for the scientific community. Moreover, the calculation of environmental costs, which are normally disregarded in a classical cost study, adds value to this study and its readers as well, as those become increasingly important for companies and society. Overall, the author concludes that the LC of SNG and hydrogen are very high in comparison with the results of peer studies, as more costs factors are considered after applying the method by Rubin et al. Besides that, the costs of fossil-produced hydrogen and natural gas are currently significantly cheaper. Furthermore, the calculation of environmental costs has clearly shown that the use of renewable energy can significantly reduce environmental impacts and thus environmental costs, which mitigates societal damage costs. As the LC of SNG and hydrogen are high, various options are available to lower the LC of SNG and hydrogen as well as to increase the costs of fossil-based processes, so that environmental impacts can be reduced and sustainably produced SNG and hydrogen become more attractive. For example, the governments subsidies of 16 billion Euros for fossil fuels could be used to reduce the electricity costs, so that sustainably produced SNG and hydrogen become cheaper. Besides that, the difference of the environmental costs between

a fossil and green process could be charged as an environmental tax on top of the production costs of the fossil process if the fossil process is cheaper. Then, fossil processes become less attractive and environmental impacts could be reduced considerably. Thus, damage costs to society could be mitigated, which is of importance in times of climate change.

Limitations

The author of the study contacted well-known manufacturers of the technologies, such as NEL ASA, Sunfire, ITM Power, etc., for data generation. Unfortunately, there was little feedback regarding the cost requests, due to confidentiality reasons, so the costs for the technologies were partly taken from the literature. This results in discrepancies since the accuracy of the manufacturers' data cannot be achieved with the help of literature values. Furthermore, the author would like to mention that the technologies under consideration are future technologies with high uncertainty factors. For this reason, high project and process contingencies have been considered, which have a significant effect on the LC.

Synopsis

Levelized and environmental costs of synthetic natural gas and hydrogen generation, considering various power-to-gas technologies and energy scenarios.

Author contributions

The manuscript was written and constructed only by the mentioned author. The author is not responsible for the final formatting. Thus, deviations of references, the right order of figures and tables, citation, punctuation, etc., might occur regarding the original document, for which the author bears no responsibility.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2023.01.347>.

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