RESEARCH ARTICLE

Simulation-based environmental-impact assessment of glycerol-to-hydrogen conversion technologies

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Abstract

This simulation-based comparative assessment aims to quantify the environmental and human-health impacts of greener hydrogen (H₂) production via three glycerol-based technologies, including: supercritical water reforming (SCWR), aqueous-phase reforming (APR) and autothermal reforming (ATR). The GaBi (2018 edition) life-cycle assessment (LCA) platform is used to develop cradle-to-gate product system models for these technologies and the TRACI 2.1 methodology is used to quantify their midpoint impact categories. Aspen HYSYS (v11) process-simulation software is used to generate the life-cycle inventory (LCI) primary data required to produce 1 kg of H₂ via each of the indicated glycerol-reforming technologies. Per ISO 14040:2006 reporting requirements for the LCA results interpretation step, three base case (BC) scenarios and four sensitivity scenarios (SS) are developed and quantified to compare the effects of different process electricity sources (US grid mix versus wind power) and thermal energy sources (natural gas versus biogas) on the LCA results. The high operating pressure (viz. 240 bar) of SCWR enabled assessment of the impact of in situ electricity generation to offset some of electricity required for this technology. The major insights from this research are as follows: (i) per 1 kg of produced H₂, APR reduces CO₂ emissions by ≈95% compared to ATR and by ≈92% compared to SCWR, (ii) for BC scenarios, the primary energy consumption (in MJ/kg of produced H₂) is in the following order from highest to lowest: ATR > SCWR > APR and (iii) H₂ production via glycerol APR is more environmentally sustainable than SCWR and ATR, and thus offers a promising path for greener H₂ production. Future environmental sustainability studies should focus on expanding the scope of this study to include H₂ production via water electrolysis using renewable electricity sources and via solar and nuclear-driven thermochemical water splitting.
Keywords: glycerol; hydrogen; impact categories; reforming; supercritical water; valorization

Introduction

Background

Hydrogen utilization
Currently, hydrogen (H₂) is mainly used in industrial processes rather than for energy production. The main industrial uses of H₂ include ammonia production (~54% of the overall H₂ consumption) and oil refineries (~35% of H₂ consumption). Other uses include chemicals synthesis (e.g., methanol production) and the food industry are responsible for the rest of the H₂ consumption [1]. As an energy carrier, H₂ is used for the transport sector and as a feedstock to proton exchange membrane (PEM) fuel cells for electricity production. For the latter application, in 2016, ~62 000 fuel-cell systems (equivalent to 500 MW of power) were shipped worldwide [2]. Globally, 7.2 EJ of energy from H₂ was consumed in 2013, which represents ~1.3% of the world primary energy consumption [1].

Hydrogen-production sources: fossil-based and water electrolysis
Currently, H₂-production technologies are mainly fossil-based, which leads to significant CO₂ emissions. For example, ~48% of H₂ production comes from steam-methane reforming (SMR), 30% is derived from petroleum refining and 18% is produced by coal gasification. In the USA only, ~10 million tons of annual H₂ production comes from SMR technology. Due to its fossil origin, H₂ production causes ~60 million metric tons of CO₂ emissions annually, which accounts for ~2% of the energy-related CO₂ emissions [3]. Water electrolysis, which enables H₂ production without CO₂ emissions, accounts for the remaining 4% of this greenhouse-gas (GHG) emission [1].

Need for greener H₂ production to curb CO₂ emissions
According to the US Environmental Protection Agency [3], the transportation sector was responsible for ~27% of GHG emissions in 2015 and, within this sector, commercial aircraft were responsible for ~9% of GHG emissions in 2015 [3]. The US Environmental Protection Agency (EPA) reported that light-duty internal combustion engine (ICE) vehicles were responsible for 60% of the GHG emissions attributed to the US transportation sector in 2015. As a result, hydrogen has been sought as a promising energy carrier for road transport. Direct H₂ use to replace petrol-based fuel in ICE vehicles or as a feedstock for on-board PEM fuel cells can contribute to curbing GHG emissions from this sector. Also, in situ renewable H₂ production in refuelling stations has been pursued to eliminate GHG emissions associated with H₂ transport from production sources to refuelling stations [2].

The UN Intergovernmental Panel on Climate Change (IPCC) reported that the civil aviation industry currently contributes ~2.5% of the world’s manmade CO₂ emissions [4, 5]. Over the past three decades, the annual growth of world commercial air transport has averaged ~5% and is projected to double over the next decade or two [6–8]. As the civil aviation fleet grows to meet increasing air-transport demands, the IPCC predicts that the contribution of the aviation industry to global manmade CO₂ emissions will increase to ~3% in 2050 [9]. To curb GHG emissions associated with the civilian aviation sector, there is an emerging interest in the development of regional1 hybrid electric aircraft (HEA) powered by combinations of conventional gas turbines and electric propulsion systems, comprising

1 Aircraft with 30–90 PAX (aircraft passengers), 4–15 tons of gross take-off weight and energy of 30 000–70 000 kWh.
motors powered by either batteries or PEM fuel cells [10], with the latter technology requiring H$_2$ storage on board aircraft. In addition to the emerging HEA technology, the full-electric aircraft technology remains a long-term vision of aircraft manufacturers like Airbus and Boeing. It is also worth mentioning that members of the EU aviation organizations and industry counterparts created the ‘Flightpath 2050’ vision to reduce global CO$_2$, nitrogen oxides (NOx) and noise emissions such that, by 2050, civil aircraft should pollute 75% less CO$_2$, 90% less NO$_x$, and 65% less noise [11].

The aforementioned background information explains the currently observed global efforts to pursue H$_2$ production from sustainable sources to curb GHG emissions, other gaseous air pollutants and particulate matter, all of which have adverse impacts on human health and the environment. In particular, bio-based H$_2$ production via reforming technologies seems to offer a viable alternative fuel compared to the use of petroleum-based fuels (viz. gasoline and diesel fuel) in the road transport sector and jet fuels in the aviation sector.

1 Motivation, objectives and novelty of research

1.1 Motivation

The discussion provided in the subsection on the ‘Need for greener H$_2$ production to curb CO$_2$ emission’ above together with the following rationale for selecting glycerol as the bio-based feedstock for greener H$_2$ production are the main motivators of this research:

- Glycerol is a by-product of biodiesel production via the transesterification of agricultural crops like soybeans, rapeseed, sunflower, jatropha, palm, castor, etc. [12–14]. In this chemical process, ~10 m$^3$ of glycerol is produced per 90 m$^3$ of rapeseed-derived biodiesel produced [15, 16]. In this research, we calculated ~7.5 m$^3$ of glycerol per 90 m$^3$ of soybean-derived biodiesel. According to Ciriminna et al. [17], the transesterification of vegetable oils for biodiesel production leads to ~10 kg of glycerol by-product per 100 kg of biodiesel produced.
- US biodiesel annual production is ~5.5 million m$^3$/year. In 2016, for example, the USA was the world’s biggest biodiesel producer [18].
- EU biodiesel annual production is ~12.5 million m$^3$/year [19].
- The increased production of biodiesel since 2000 to the present in both the USA and the EU led to a substantial reduction in glycerol prices.

In this author’s opinion, glycerol-reforming technologies offer a promising bio-based H$_2$ source, in particular aqueous-phase reforming (APR), which could ultimately replace the current use of SMR technology, which emits ~11 kg CO$_2$-equiv. per kg of H$_2$ produced [14]. In this regard, CO$_2$ emission associated with glycerol feedstock is expected to be low because, while this GHG is emitted during biomass cultivation, pretreatment, oil extraction and refining, the transesterification process and glycerol-purification steps, CO$_2$ is also absorbed during biomass farming, hence reducing the net emissions of CO$_2$.

1.2 Objective

This research aims to perform comparative assessments of energy consumption, environmental burdens and adverse human-health impacts of glycerol-based H$_2$ production via the three reforming technologies, viz. supercritical water reforming (SCWR), APR and autothermal reforming (ATR), respectively. To achieve this objective, life-cycle impact assessment (LCIA) is performed for base case (BC) scenarios in which the US electricity-grid mix is assumed to be the electricity supply source to power pumps and compressors in the reforming processes. The US grid electricity mix [20] is as follows: 39.5% natural gas, 23% coal, 20% nuclear and 17.5% renewables (of which 7.2% is wind power, 6.4% hydropower, 1.7% solar, 1.3% biomass and 0.4% geothermal). Also, natural-gas burning is assumed to supply the thermal energy required for the reformer and for heating the reactant mixtures to the required reforming temperature. LCIA is also performed for sensitivity scenarios in which wind power is assumed to be the electricity source instead of the electricity-grid mix and biogas burning instead of natural gas to supply the thermal energy of reformers. Additionally, optimization strategies to reduce reforming energy requirements (both electrical and thermal) are also considered in the LCIA assessment scenarios.

1.3 Novelty

Unlike previous investigations that focused only on estimating the carbon footprint associated with a single glycerol-reforming technology, this research addresses current voids in the state of knowledge about the three selected glycerol-reforming technologies by providing the following quantitative insights:

- comparative energy consumption and midpoint impact categories among these reforming technologies;
- efficient energy-management strategies for these reforming technologies. These strategies include: (i) capturing exothermic heat from the reforming reaction steps, (ii) burning exhaust combustible gases to offset the endothermal heat of the reformer and (iii) for SCWR technology, which is energy-intensive due to the high-pressure requirement, the electricity-generation option in conjunction with H$_2$ production has been evaluated.

The remaining sections of this manuscript are organized as follows. Section 2 discusses the key findings of the relevant published work, Section 3 presents the adopted research methods and tools, and Section 4 discusses the results of this environmental sustainability assessment.
The principal results and major conclusions of this research are summarized in Section 5.

2 Literature review

This research focuses on bio-based greener H₂ production via glycerol reforming technologies and, hence, the scope of this literature review is limited to achieving this purpose. The three glycerol-based technologies being considered herein are: SCWR, APR and ATR. Glycerol is a by-product of biodiesel production via the transesterification of agricultural crops. (More details and statistical data about this feedstock are provided in Section 1.1).

The remainder of this subsection provides brief highlights of key published research on H₂ production via glycerol reforming. Wen et al. [21] studied the activities and stabilities of Pt, Ni, Co and Cu catalysts and their support substrates for H₂ production via APR of glycerol. Authayanun et al. [22] investigated the thermodynamics of H₂ production via ATR of crude glycerol derived from the biodiesel-production processes. They assumed glycerol and methanol to be the primary components of the crude glycerol and found that H₂ production increases as the ratio of glycerol to methanol increases and as the reforming temperature increases. Ortiz et al. [23] performed thermodynamic analysis of the glycerol SCWR process using AspenPlus™ and used the Soave-Redlich-Kwong (SRK) equation of state to identify the thermodynamically favourable operating conditions for glycerol conversion to H₂. They used from 1 to 16 mol % (≈5–50 wt%) of glycerol concentration in the feed stream, with water being the balance, and conducted SCWR at 240 bar and 800°C. Zhang et al. [24] provided characterization of the Pt–Re catalysts under conditions encountered during APR to obtain an improved understanding of the role of the Rhenium (Re) catalyst. Their results showed the importance of surface acidity in controlling the reaction pathways during glycerol APR. Ortiz et al. [25] simulated glycerol SCWR to produce H₂ and electricity. Avasthi et al. [26] focused their research on the glycerol/steam reforming (GSR) technology and discussed current challenges (e.g. higher prices of biodiesel compared to diesel fuel) and potential solutions. In this author’s opinion, none of the proposed solutions (e.g. in situ removal of CO₂ and H₂ as soon as they form inside the reformer) seems to be practical.

Rocha et al. [12] used a cradle-to-gate (C2G) life-cycle assessment (LCA) approach to quantify the environmental and health impacts of the production of biodiesel from soybean and palm oil. Their analysis was performed using SimaPro software and CML 2000 LCA methodology. Galera and Ortiz [14] evaluated the environmental performance of H₂ and electricity production via glycerol SCWR. They used SimaPro 8.0. CML 2000 in their LCA study and estimated that ≈3.77 kg CO₂-eqiv/kg H₂ was produced after taking credit for their assumption of biogenic versus fossil-based CO₂ emissions. Rahman [27] investigated 1 wt% glycerol (in DI water) APR over a series of nickel (Ni) and copper–nickel (Cu–Ni) bimetallic catalysts supported on multiwalled carbon nanotubes (MWNT) at 240°C and 40 atmospheres. His test results showed that the Cu–Ni catalyst led to 86% H₂ selectivity and 84% glycerol conversion, and noted that the presence of Cu in bimetallic catalysts led to the suppression of undesirable methanation reactions. Subramanian et al. [16] studied glycerol APR over a series of γ-Al₂O₃-supported metal nanoparticle catalysts for H₂ production in a batch reactor. They found that Pt/Al₂O₃ was the most active catalyst under the test conditions. The optimum conditions for H₂ production were found to be 240°C, 42 bar, 1000 r.p.m. stirring speed and ≈4100 substrate/molar ratio for a 10-wt% glycerol feed.

Schwenger et al. [19] published a review paper on glycerol reforming and highlighted key characteristics of the reported technologies. Larimi et al. [28] synthesized a series of M-doped Pt/MgO (where M could be palladium, ruthenium, rhodium, iridium or chromium) nano-catalysts and examined their performance effects on glycerol APR. Boga et al. [29] investigated the effect of individual components of crude glycerol on APR activity over 1 wt% Pt/Mg(Al)O, 1 wt% Pt/Al₂O₃, 5 wt% Pt/Al₂O₃ and 5 wt% Pt/C catalysts at 29 bar and 225°C. The use of a 10-wt% alkaline crude glycerol solution in water, containing 6.85 wt% glycerol, 1.62 wt% soaps, 1.55 wt% methanol and 0.07 wt% ester, caused a noticeable drop in APR activity compared to the corresponding 6.85-wt% solution of pure glycerol in water.

Most recently, Veluturla et al. [30] discussed the use of different types of heterogeneous catalysts for glycerol valorization through processes like carboxylation, condensation, esterification, etherification, phase reformation, selective oxidation, hydrolysis transesterification, selective reduction and pyrolysis. Putra et al. [31] performed glycerol APR and phenol hydrogenation with Raney Ni at 180–240°C for phenol-to-glycerol ratios from 0 to 4.88. They selected phenol as a model lignin monomer to demonstrate the feasibility of using renewable H₂ from glycerol APR for lignin upgrading. Ghani et al. [32] reformed crude glycerol over modified cerium–zirconium (Ce–Zr) supports loaded with 5 wt% nickel catalyst to generate H₂ via ATR (a combination of partial oxidation and steam reforming). They studied the effects of the reforming temperature, steam-to-carbon ratio (S/C), oxygen-to-carbon ratio (O/C), reduction temperature and calcination temperature, and reported the following optimum operating conditions: a reforming temperature of 550°C, S/C of 2.6, O/C of 0.5, reduction temperature of 600°C and calcination temperature of 550°C. Bastan et al. [33] investigated the effects of the Al/Mg ratio in a series of Ni nano-catalysts supported on Al₂O₃ and MgO on the physico-chemical characteristics of Ni/Al₂O₃–MgO catalysts and determined the optimum catalyst for H₂ production via glycerol APR. They found that the APR activity of synthesized catalysts strongly depended

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2 Platinum–rhenium catalyst.
on the Al/Mg ratio and demonstrated that the Ni/Al\(_2\)Mg catalyst possessed the highest catalytic activity of 92% glycerol conversion and selectivity towards a hydrogen production of 76%. Charisiou et al. [34] investigated the GSR reaction for H\(_2\) production and compared the performance of Ni supported on ZrO\(_2\) and SiO\(_2\)–ZrO\(_2\) catalysts. They suggested that the addition of SiO\(_2\) stabilizes the ZrO\(_2\) monoclinic structure, restricts the sintering of Ni particles, strengthens the interaction between Ni\(^{2+}\) species/support and influences the distribution of the gaseous products by increasing the H\(_2\) yield (while not favouring the transformation of CO\(_2\) to CO). Thus, a high H\(_2\)/CO ratio can be achieved with a negligible CO/CO\(_2\) ratio. Shejale and Yadav [44] investigated the GSR and compared two catalysts, viz. Ni–Cu/La\(_2\)O\(_3\)–MgO and Ni–Co/La\(_2\)O\(_3\)–MgO, prepared by the co-precipitation and impregnation techniques for the GSR reaction.

With respect to the valorization of glycerol to produce value-added products, Kaur et al. [39] provided a comprehensive assessment for the production of value-added products from crude glycerol. Their assessment included the environmental and economic aspects of different glycerol-conversion routes such as the chemical and biochemical methods.

### 3 Methods
Sections 3.1 and 3.2 present the methods and tools employed in this research. Section 3.3 presents the roadmap for integrating Aspen HYSYS simulation results into GaBi\(^4\) product system models to calculate environmental burdens and human-health impacts, and Section 3.4 provides life-cycle inventory (LCI) primary data generated using Aspen HYSYS simulations of SCWR, APR and ATR technologies.

#### 3.1 LCA
This research follows the LCA methodology described in ISO 14040:2006 standards [40]. The LCA methodology comprises four interrelated steps as follows [8, 35]:

(i) Goal and scope definition step that also includes specifying the boundaries of the system being analysed and defining the functional unit (FU). The goal here is to conduct a quantitative environmental sustainability assessment to identify which, among three glycerol-reforming technologies, would be characterized as the most sustainable and environmentally friendly technology for greener H\(_2\) production. The scope is about H\(_2\) production from glycerol feedstock and, hence, the system boundary is denoted as a cradle-to-production gate (C2P) boundary (Fig. 1). Finally, the selected FU is assumed to be 1 kg of produced H\(_2\).

(ii) LCI analysis that includes input/output materials and energy flows and direct emissions. During this step, the process input/output mass and energy flows as well as compositions are calculated and data gaps are identified. In this regard, LCI data fall into two categories: primary (viz. foreground) and secondary (viz. background) data. In this research, the primary data for each of the three glycerol-reforming technologies is produced using Aspen HYSYS process simulation. The secondary data (such as the environmental and human-health burdens associated with the glycerol by-product of biodiesel production via the transesterification of biomass) is directly obtained from the GaBi LCI database.

(iii) LCIA, where the environmental burdens of the material and energy flows as well as human-health impacts are quantified. The impact assessment of interest to this research focuses on human health and the natural environment. As discussed in Khalil [8, 35] as well as in the ILCD Handbook [36], there are many methodologies for conducting LCIA such as CML 2002, Eco-Indicator 99, EPS 2000, Impact 2002+, ReCiPe 2008, USEtox, TRACI, etc. However, we selected to adopt the TRACI methodology that is currently used in the GaBi LCA software package. Also, the midpoint characterization methodology has lower uncertainty in the results compared to the endpoint characterization used in other methodologies such as Eco-Indicator 99 [37]. The author of this work...

![Fig. 1: System boundary of the cradle-to-gate (hydrogen-production plant) system](https://academic.oup.com/ce/article-5/3/387/6317702/7)

\(^4\) GaBi ThinkStep LCA platform. Source: [http://www.gabi-software.com](http://www.gabi-software.com).

\(^5\) TRACI: A Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts.
also used TRACI LCIA methodology in his previous research [8, 35].

TRACI 2.1 LCIA methodology—the US EPA developed the impact-assessment methodology (viz. TRACI) for the purpose of LCA studies [38]. The impact categories are characterized at the midpoint level draw simple cause–effect chains to show the point at which each impact category is characterized and reflect the current state of developments, consistently with EPA regulations and policies, as well as the best available LCIA practices. The impact categories used in the TRACI methodology are shown in Table 1. The GaBi platform includes TRACI 2.1 (which is the latest version of this database).

(iv) Interpretation of the analysis results including sensitivity studies and scenarios analysis. In this research, three BC scenarios and four sensitivity scenarios are developed and analysed, as discussed in Section 4.

As Table 1 shows, there are two impact categories that directly refer to human health, namely the carcinogens and non-carcinogens impact categories. However, other impact categories also affect human health, such as particulate matter, smog formation, ozone depletion and global warming [37]. Also, NOx emissions are represented in the eutrophication and acidification impact categories. Note that SOx and NOx are contributors to acid gases, which are represented in the acidification potential (measured in kg SO2-equiv.).

In this research, the GaBi LCA tool (2018 edition) has been used to develop C2G product system models for the glycerol-reforming technologies being evaluated. GaBi product system models account for the environmental and human-health burdens associated with glycerol (a by-product of the biodiesel process), which is an input feed stream to GaBi product system models.

3.1.1 Process design and simulation

The use of Aspen HYSYS is deemed necessary to simulate each of the three glycerol-reforming technologies and provide useful quantitative information including input/output mass and energy flows per 1 kg of produced H2, compositions of gaseous and liquid process streams, pressure and temperature conditions of the input and output streams, as well as operating conditions inside the simulated unit operations (viz. reformer, water–gas shift (WGS) reactors, gas/liquid separator and pressure-swing adsorber). The Aspen HYSYS CPA fluid property package has been selected for performing the thermodynamic calculations in the simulated glycerol-reforming technologies.

Aspen HYSYS simulations also allowed modelling energy-management strategies such as capturing exothermic heat from some of the reforming reaction steps and from burning exhaust combustible gases to offset the overall endothermic heat of the reformer. For SCWR technology, which is energy-intensive due to the high-pressure requirement, the in situ electricity-generation option in conjunction with H2 production has been evaluated using Aspen HYSYS simulation.

3.1.2 Integration of process simulation with LCA models

Because GaBi LCI databases do not contain LCI data for the bio-based production of H2 from glycerol via SCWR, APR or ATR, it was necessary to use the Aspen HYSYS platform to simulate each of the three reforming processes. Fig. 1 shows the HYSYS simulation of the APR process. HYSIS simulations of the SCWR and ATR have unit operations similar to those shown in Fig. 1. However, the main differences among the three HYSIS simulations include the operating conditions and feed streams of the reformer. For example, SCWR uses supercritical water and glycerol, and ATR uses air (in addition to water and glycerol) in the reformer.

Description of the unit operations depicted in Fig. 2. A mixer is used to blend the glycerol and water (in the required weight percentages), a pump to compress the feed mixture to the desired operating pressure of the reformer and a heat exchanger to heat the feed to the desired operating temperature of the reformer. Downstream of the reformer is an expander valve to lower the pressure of the product gases followed by a heat exchanger (Heater-1) upstream of the high-temperature gas–water shift reactor (GWS-1). The latter unit operation is followed by a cooling heat exchanger (Cooler-1) to lower the temperature of the gases before entering the low-temperature WSG-2.

The gaseous stream leaving the WGS-2 is then cooled in Cooler-2 before entering the gas separator, which separates the gases from condensed water. A pressure-swing absorber unit is used to separate the product H2 from other combustible gases (a mixture of CO and some H2 and CO2). The heat generated from the combustion of CO and remaining H2 is used to offset the heat required for the glycerol reformer. The stream of exhaust gases is then cooled (in Cooler-3) before it goes to the stack.

Table 1: TRACI 2.1 midpoint impact categories

| TRACI 2.1 midpoint impact category | Units   |
|-----------------------------------|---------|
| Acidification                     | kg SO2-equiv. |
| Ecotoxicity                       | CTUe    |
| Eutrophication                    | kg N-equiv. |
| Global warming                    | kg CO2-equiv. |
| Human-health particulate matter   | kg PM2.5-equiv. |
| Human toxicity, carcinogens       | CTUh    |
| Human toxicity, non-carcinogens   | CTUh    |
| Ozone depletion                   | kg CFC 11-equiv. |
| Smog formation                    | kg O3-equiv. |

CTUe, comparative toxic unit for ecotoxicity impacts (e.g. freshwater toxicity); CTUh, comparative toxic unit for human-toxicity impacts.

 CPA = Cubic-Plus-Association equation of state.
The three glycerol-reforming processes (SCWR, APR and ATR) for H₂ production involve the following primary and secondary stoichiometric reactions:

R1: Glycerol reforming (primary reaction)
\[ C_3H_8O_3 + 3H_2O \rightleftharpoons 7H_2 + 3CO_2 \] (ΔH)ₚ at 25°C = 127.75 KJ/mole

In addition to the primary reforming reaction (R1), secondary reactions may also occur (as described by R2 and R3).

R2: Methanation reaction
\[ CO + 3H_2 \rightleftharpoons CH_4 + H_2O \] (ΔH)ₚ at 25°C = -205.88 KJ/mole

R3: Methane dry reforming reaction
\[ CO_2 + CH_4 \rightleftharpoons 2H_2 + 2CO \] (ΔH)ₚ at 25°C = 247.02 KJ/mole

R4: Glycerol-oxidation reaction (unique to the ATR process)
\[ C_3H_8O_3 + 1.5O_2 \rightleftharpoons 3CO_2 + 4H_2 \] (ΔH)ₚ at 25°C = -597.73 KJ/mole

High-temperature (350°C) and low-temperature (200°C) WGS reactors are included in the three reforming processes to convert CO (in the presence of H₂O) into CO₂ and H₂.

R5: WGS reaction
\[ CO + H_2O \rightleftharpoons CO_2 + H_2 \] (ΔH)ₚ at 25°C = -41.14 KJ/mole

Note: Calculations of the reaction enthalpies at 25°C and 1 a.t.m. are performed using HSC Chemistry® software (version 10) [42].

Fig. 2: Reforming process simulation of the aqueous-phase reforming technology for hydrogen production

Fig. 3 shows how Aspen HYSYS results are integrated with GaBi product system models to quantify...
the environmental burdens and adverse human-health impacts of each of the three glycerol-based hydrogen-production technologies.

For both Aspen HYSYS simulations and GaBi product system models, 1 kg of H\textsubscript{2} produced has been selected as the FU. Hence, all mass and energy flows and mid-term impact categories are calculated per 1 FU of produced H\textsubscript{2}.

### 3.1.3 LCI primary data

The three glycerol-reforming technologies (SCWR, APR and ATR) are simulated using the Aspen HYSYS platform to generate the LCI primary data required as the input to GaBi product system models. The primary data for SCWR, APR and ATR are provided in Tables 2, 3 and 4, respectively.

### 4 Results and discussion

The following subsections present results of Aspen HYSYS simulations and GaBi LCIA for the three selected glycerol-reforming technologies for H\textsubscript{2} production. Also discussed is the interpretation of the generated results. Per ISO 14040:2006 [40], the interpretation step of the LCA
framework requires that the assessment results should be reported by the most informative means possible. In light of this ISO reporting requirement, this research adopts the following approaches for interpretation of its LCIA numerical results, namely: (i) BC comparative assessments of TRACI 2.1 LCIA results per impact category across the selected bio-based H₂-production technologies; (ii) sensitivity scenarios that quantify the effect on the calculated midpoint impact categories as a result of variations in process electricity sources (viz. US electricity-grid mix versus wind power) and thermal energy sources (viz. natural gas versus biogas). Moreover, the distinctively high operating

Table 3: Primary life-cycle inventory data associated with the aqueous-phase reforming (APR) of glycerol for 1 kg of H₂ production

| Mass and energy inputs | Mass and energy outputs |
|------------------------|-------------------------|
| Glycerol feedstock: 7.7 kg | H₂ gas: 1 kg |
| Water to reformer: 69.3 kg | CO₂ gas: 955 kg |
| Air to combustible-gases furnace: 0.123 kg | Water: 65.4 |
| Water/glycerol mass ratio = 9.0 | Stack emissions: 1.173 kg |
| Reformer operation conditions: | • CO gas: 0.051 kg |
| • Temperature: 290°C | • Water vapour: 0.972 kg |
| • Pressure: 52.69 bar | • N₂ gas: 0.0943 kg |
| Total mass in: 77.123 kg | • CH₄ gas: 0.056 |
| Thermal energy required = 216.67 MJ | Total mass out: 77.123 kg |
| Electrical energy required = 0.522 MJ | Thermal energy available for harvesting at 90% thermal efficiency = 201.08 MJ |
| (to operate process pumps/compressors) | Net thermal energy required is ≈16.11 MJ assuming credit is given to the thermal energy available for harvesting |

Table 4: Primary life-cycle inventory data associated with the autothermal reforming (ATR) of glycerol for 1 kg of H₂ production

| Mass and energy inputs | Mass and energy outputs |
|------------------------|-------------------------|
| Glycerol feedstock: 9.21 kg | H₂ gas: 1 kg |
| Water to reformer: 4.33 kg | CO₂ gas: 8.81 kg |
| Air to combustible-gases furnace: 5.53 kg | Water: 2.07 |
| Water/glycerol mass ratio = 0.47 | Stack emissions: 7.19 kg |
| Reformer operation conditions [43]: | • CO gas: 0.0997 kg |
| • Temperature: 650°C | • Water vapour: 0.0 kg |
| • Pressure: 1.013 bar | • N₂ gas: 4.24 kg |
| Total mass in: 19.07 kg | • CH₄ gas: 2.85 |
| Electrical energy required = 41.1 MJ | Total mass out: 19.07 kg |
| (to operate process pumps/compressors) | |
| If credit is given to thermal-energy harvesting (at 90% efficiency) in the ATR process, it would be sufficient to offset the thermal energy required for the reformer |

Fig. 4: Product system model for H₂ production using glycerol SCWR Input and output mass and energy data for the SCWR technology are presented in Table 2.
pressure (240 bar) of the SCWR technology allowed for analysing the effect of \textit{in situ} electricity generation to offset some of the required electricity on the LCIA impact categories.

4.1 Aspen HYSYS simulations: BC and SS

To meet the research objectives discussed in Section 2.2, Aspen HYSYS models are developed to simulate the following glycerol-reforming scenarios: (i) BC scenarios in which the US electricity-grid mix is assumed to supply the electrical power to operate the pumps and compressors in the glycerol-reforming processes; also, natural-gas burning is assumed to supply the required reformer’s thermal energy and for heating the reactants to the required reforming temperature; (ii) SS in which wind power, instead of the electricity-grid mix, is assumed to supply the electrical power for the process pumps and compressors, and biogas burning, instead of natural gas, to supply the thermal energy required for the reformer; (iii) optimization strategies to reduce the reforming energy requirements (both electrical and thermal) are also considered in the HYSYS simulations. More details about the energy-optimization strategies are discussed in Section 4.2.

The mass and energy flows calculated using Aspen HYSYS to produce 1 kg H\textsubscript{2} are provided in Tables 2, 3 and 4, respectively. Also, with respect to SCWR of glycerol, Khalil [35] estimated that \( \sim 79 \text{ MJ} \) of energy would be required to produce 1 kg of supercritical water (SCW). This energy is consumed in heating the water to temperatures above its critical point (374\textdegreeC) and compressing the resulting steam to pressures above its critical pressure (220 bar).

4.2 Quantifications of GaBi LCA product system models for H\textsubscript{2} production

4.2.1 SCWR for H\textsubscript{2} production

Fig. 4 shows the input and output streams of the GaBi product system model for the production of 1 kg of H\textsubscript{2} (i.e. 1 FU) using SCWR technology. Input and output mass and energy data are presented in Table 2. The input mass streams represent the glycerol and water feedstocks. The input energy streams include the thermal energy required by the reformer and electricity (from the US grid mix) to...
provide the electrical power to the process pumps and compressors. It is assumed that diesel-powered trucks are used for the transportation of glycerol from the biodiesel plant to the reforming plant (distance is assumed to be 50 km). The output streams include H₂, gaseous emissions (N₂, CH₄, CO₂, etc.) and water removed by the gas/liquid separator. These unit operations were modelled in Aspen HYSYS simulations (as illustrated in Fig. 2).

The reformer is modelled by a conversion reactor (at 800°C and 240 bar) and the two WGS reactors (WGS-1 and WGS-2) are modelled by equilibrium reactors. WGS-1 operates at 350°C and 15 bar and WGS-2 operates at 200°C and 15 bar.

Table 5 provides the nine TRACI 2.1 midpoint impact categories associated with the production of 1 FU (viz. 1 kg) of H₂ using SCWR for Scenarios 1 and 2, respectively.

The results summarized in Table 5 indicate some reductions in the burdens associated with human health and the environment as a result of generating electrical power (by expanding the hot exhaust gases from the reformer through an installed turbine) to offset the electric loads required to operate the process pumps/compressors. The associated global-warming potential is 51.9 kg CO₂-equiv. for Scenario 1 and 51.5 kg CO₂-equiv. for Scenario 2. Clearly, this energy-management strategy led to an ≈0.8% carbon-footprint reduction (namely 0.4 kg CO₂-equiv. per kg of produced H₂). In both scenarios, the biogenic carbon represents ≈27% of the associated global warming potential (GWP) (measured in kg CO₂-equiv. per kg of H₂ produced). As Table 3 shows, the highest impact category reduction is related to ozone depletion (=81%) and the lowest impact reduction is related to the eutrophication (=0.2%) impact category. The reduction in the human-toxicity (non-carcinogenic) impact category is ≈23%.

4.2.2 APR for H₂ production

Fig. 5 depicts the input and output streams of the GaBi product system model for the production of 1 kg of H₂ using APR technology. The input mass streams include glycerol and water feedstocks. The input energy streams include thermal energy required by the reformer and the two WGS reactors. Table 6 presents the detailed results of the TRACI 2.1 midpoint impact categories for Scenarios 3, 4, and 5.

Table 6: Midpoint impact categories associated with aqueous-phase reforming (APR) of glycerol for 1 kg of H₂ production

| TRACI 2.1 midpoint impact categories | Scenario 3a | Scenario 4b | Scenario 5c |
|-------------------------------------|-------------|-------------|-------------|
| Acidification (kg SO₂-equiv.)        | 2.08 × 10⁻³ | 9.66 × 10⁻³ | 1.83 × 10⁻³ |
| Ecotoxicity (CTUe)                   | 6.46 × 10⁻² | 1.25 × 10⁻¹ | 6.28 × 10⁻¹ |
| Eutrophication (kg N-equiv.)         | 3.19 × 10⁻⁴ | 2.76 × 10⁻⁴ | 3.06 × 10⁻⁴ |
| Global warming (kg CO₂-equiv.)       | 4.11        | 4.18        | 3.88        |
| Human-health particulates (kg PM2.5-equiv.) | 2.74 × 10⁻⁴ | 5.00 × 10⁻⁴ | 2.55 × 10⁻⁴ |
| Human toxicity, carcinogenic (CTUh)  | 7.59 × 10⁻¹⁰| 2.00 × 10⁻⁹ | 7.45 × 10⁻¹⁰|
| Human toxicity, non-carcinogenic (CTUh) | 1.76 × 10⁻⁸  | 3.93 × 10⁻⁷ | 1.65 × 10⁻⁷ |
| Ozone depletion (kg CFC 11-equiv.)   | 4.96 × 10⁻¹⁰| 5.53 × 10⁻¹¹| 1.46 × 10⁻¹¹|
| Smog (kg O₃-equiv.)                  | 1.03 × 10⁻¹  | 1.56 × 10⁻¹ | 1.01 × 10⁻¹ |

aScenario 3: This is the base case scenario in which natural gas is used to provide the required thermal energy in the process. The US electricity-grid mix provides the required process electricity.
bScenario 4: In this scenario, biogas is used instead of natural gas to provide the required thermal energy for the process. The US electricity-grid mix provides the required process electricity.
cScenario 5: In this scenario, wind-turbine power is used instead of the electricity-grid mix as the source of electricity for operating the process compressors and pumps.
Inspection of the results depicted in Table 6 shows that, in the sensitivity scenario, electrical power is assumed to be provided from wind power. Table 7 summarizes the GaBi LCIA results (midpoint impact categories associated with the production of 1 kg of H₂ using ATR technology).

As Table 7 shows, switching the electricity supply from the US grid mix to wind power resulted in a substantial reduction in the adverse environmental impacts (with the exception of water eutrophication). Also, the carbon-footprint reduction is ~8%. The notably higher value of the eutrophication potential compared to APR (see Table 5) and SCWR (see Table 3) can be attributed to use of air in the ATR reformer and the resulting N₂ emissions (as shown in Tables 2, 4 and 6, respectively).

### 4.3 Environmental sustainability assessment

In alignment with ISO 14040:2006 [40] reporting requirements for the LCA results interpretation step, Sections 4.2.1, 4.2.2 and 4.2.3 presented the LCIA results for SCWR, APR and ATR technologies and compared their associated environmental impacts. The notable higher value of the eutrophication potential compared to APR (see Table 5) and SCWR (see Table 3) can be attributed to use of air in the ATR reformer and the resulting N₂ emissions (as shown in Tables 2, 4 and 6, respectively).

### Table 8: Comparative primary energy consumption to produce 1 kg of H₂ gas via glycerol reforming

| Glycerol-reforming technology | Primary energy consumption (MJ/kg H₂) |
|------------------------------|--------------------------------------|
| Supercritical water reforming (SCWR): | |
| • Scenario 1, viz. (BC)SCWR | 33.17 |
| • Sensitivity Scenario 2 (SS-2) | 27.68 |
| Aqueous-phase reforming (APR): | |
| • Scenario 3, viz. (BC)APR | 23.76 |
| • Sensitivity Scenario 4 (SS-4) | 23.71 |
| • Sensitivity Scenario 5 (SS-5) | 23.62 |
| Autothermal reforming (ATR): | |
| • Scenario 6, viz. (BC)ART | 121.15 |
| • Sensitivity Scenario 7 (SS-7) | 104.43 |

4.2.3 ATR for H₂ production

Fig. 6 shows the input and output streams of the GaBi product system model for the production of 1 kg of H₂ (i.e. 1 FU) using ATR technology. Input and output mass and energy data are presented in Table 6. The input mass streams represent glycerol and water feedstocks as well as air for the ATR reformer. The input energy streams include the thermal energy required by the reformer, the US electricity grid to provide electrical power to process pumps and compressors, and US diesel-powered trucks for the transportation of glycerol from the biodiesel plant to the reforming plant (assumed to be 50 km). The output streams include H₂, gaseous emissions (N₂, CH₄, CO₂, etc.) and water removed to the gas/liquid separator. The ATR reformer is modelled by a conversion reactor (at 650°C and 1.013 bar) and the two WGS reactors (WGS-1 and WGS-2) are modelled by equilibrium reactors. WGS-1 operates at 350°C and 15 bar and WGS-2 operates at 200°C and 15 bar.

Input and output mass and energy data for the ATR technology are presented in Table 6.

The reformer is modelled by a conversion reactor (at 290°C and 52.69 bar) and the two WGS reactors (WGS-1 and WGS-2) are modelled by equilibrium reactors. WGS-1 operates at 350°C and 15 bar and WGS-2 operates at 200°C and 15 bar. Input and output mass and energy data for the APR technology are presented in Table 6.

In the BC scenario, electrical power is provided from the US electricity-grid mix. In the sensitivity scenario, electrical power is assumed to be provided from wind power.
BC scenarios versus sensitivity scenarios with respect to environmental and human-health impacts. Section 4.3 shows how the aforementioned LCIA results (viz. sustainability indicators) of SCWR, APR and ATR compare with each other in order to identify which glycerol-reforming technology can be considered the most sustainable. The indicators of this environmental sustainability assessment are: primary energy consumption and environmental and human-health impacts (all evaluated per 1 kg of produced H₂). Table 8 summarizes the primary energy consumed to produce 1 kg of H₂ for the BC scenarios as well as the SS.

As Table 8 shows, the primary energy consumptions (measured in MJ/kg of produced H₂) of the three BC scenarios can be ordered (from highest to lowest) as follows:

ATR > SCWR > APR

Accordingly, APR represents the lowest energy-intensive glycerol-reforming technology compared to ATR and SCWR. As shown by the three BC scenarios in Table 8, the energy intensity (MJ/kg H₂) of APR is ≈20% of that associated with ATR and ≈72% of that associated with SCWR. Also, it should be noted that the ATR process has three feed streams entering the reformer (glycerol, water and air), which have to be heated to the reformer operating temperature of 650°C. Hence, as Table 8 shows, there is more primary energy consumption (in MJ/kg H₂) in the ATR process compared to the SCWR and APR processes.

As a benchmark, Spath and Mann [45] reported 183.2 MJ/kg H₂ for the primary energy consumption of SMR technology.

Other quantitative insights from Table 8 (three BC scenarios and four SS):

- For SCWR: in situ electricity generation (via expanding the high-pressure product gases from the reformer) to offset the use of electricity from the grid mix resulted in an ≈17% reduction in primary energy consumption per kg of produced H₂.
- For ATR: use of electricity from wind power instead of electricity from the US grid mix resulted in an ≈14% reduction in the primary energy consumption per kg of produced H₂.
- For APR: replacement of natural gas with biogas as the source of thermal energy for the reforming process led to an ≈0.21% reduction in primary energy consumption compared to the BC scenario in which natural gas (NG) is the source of thermal energy for the reformer. Also, the use of wind power instead of grid mix to provide the electricity required to power the compressors and pumps in the APR process led to an ≈0.60% reduction in the primary energy consumption per kg of produced H₂.

Figs 7–9 compare the nine TRACI 2.1 midpoint impact categories of the three BC scenarios associated with the SCWR, APR and ATR processes for glycerol-based H₂ production. The impact categories are divided among Figs 7–9 for visual clarity purposes (notice the y-axis scale differences). The general trends in the three figures show that the impact categories are highest for ATR, lowest for APR, with SCWR somewhere in between.
A closer inspection of Fig. 7 shows that the APR process leads to the highest reduction in the eutrophication category (followed by SCWR) compared to ATR. Quantitatively, the eutrophication impact category associated with APR technology is <0.01% of that associated with ATR technology and ≈2% of that associated with SCWR technology. The notably high eutrophication category associated with ATR can be attributed primarily to the air used in the reformer and the resulting N₂ emission.

A closer inspection of Fig. 8 shows that the APR process leads to the highest reduction in ozone depletion (followed by SCWR) compared to ATR.

Inspection of Fig. 9 for BC scenarios shows that the APR technology reduces CO₂ emissions by ≈95% per kg of produced H₂ compared to ATR and by ≈92% per kg H₂ compared to SCWR. As a benchmark, CO₂ emission from SMR is 11.9 kg CO₂-eq./kg H₂ [45] compared to 4.1 kg CO₂ equiv./kg of H₂ for the APR technology. However, the CO₂ emission...
from SMR remains below that of the ATR and SCWR technologies (which are 87.2 and 51.9 kg CO₂ equiv./kg H₂, respectively).

Additional quantitative LCIA-based insights:

- SCWR sensitivity Scenario 2 shows a reduction of ≈0.4 kg CO₂-equiv./kg H₂ compared to SCWR Scenario 1 (BC) as a result of using in situ generated electricity compared to using electricity from the US grid mix to power the process pumps and compressors in the SCWR process.
- APR sensitivity Scenario 4 shows a carbon-footprint reduction of ≈0.7 kg CO₂-equiv./kg H₂ as a result of using wind power (a renewable energy source) instead of the US electricity-grid mix (BC Scenario 3) to power the process pumps and compressors in the APR system.
- ATR sensitivity Scenario 7 shows a reduction in the carbon footprint of ≈6.9 kg CO₂-equiv./kg H₂ as a result of using wind power, instead of grid electricity, to power the process pumps and compressors in the ATR process.

It is this author’s opinion that bio-based H₂ production via glycerol APR technology is a promising alternative to fossil-based H₂ production using SMR for the following reasons:

- SMR technology consumes natural gas (a depletable resource) and emits ≈11.9 kg CO₂ for every kg of produced hydrogen. It should be noted that this CO₂ emission from SMR is fossil-based as opposed to being biogenic CO₂.
- SMR is an energy-intensive technology and would be even more energy-intensive if the SMR plant is integrated with carbon-capture and sequestration processes.
- Glycerol feedstock in APR is a by-product of biomass transesterification to produce biodiesel. Also, glycerol APR technology emits ≈4.11 kg CO₂ per kg of produced H₂ compared to ≈11.9 kg CO₂ based on the SMR technology.
- The carbon footprint of the APR technology can be further reduced by integrating the bio-based hydrogen product plant with the biodiesel plant to eliminate GHG emissions associated with glycerol transport.

5 Conclusions

The future of hydrogen as an energy carrier is important, but so too is the ability to quantify the energy requirements and environmental burdens associated with H₂ production technologies. In this regard, LCA is a central framework for performing comparative environmental sustainability analyses of H₂ production technologies.

Production of H₂ from bio-based feedstocks such as glycerol (a by-product of biodiesel production via biomass transesterification) is considered a carbon-neutral technology because its associated CO₂ emission is assumed to be absorbed during the growth phase of the plant.

In this study, we carried out an environmental sustainability assessment of glycerol reforming for H₂ production using a quantitative methodology that integrated Aspen HYSYS process simulations with the GaBi LCA platform. The sustainability indicators used in this assessment conform to the TRACI 2.1 LCIA methodology and include the primary energy consumption and midpoint impact categories (viz. human-health and environmental impacts) per kg of H₂.

The results of our study revealed that H₂ production from glycerol via APR is more environmentally sustainable than glycerol ATR, SCWR and conventional SMR technology. For example, the primary energy consumption (in MJ/kg H₂) can be ranked from highest to lowest in the following order of H₂ production technologies: SMR > ATR > SCWR > APR. The associated CO₂ emissions (in kg CO₂-equiv./kg H₂) can also be ranked from highest to lowest in the following order of H₂ production technologies: ATR > SCWR > SMR > APR.

Future research should focus on expanding the scope of this comparative environmental assessment to include other H₂ production routes such as water electrolysis using electricity from wind turbines and solar photovoltaic, as well as the nuclear-powered and solar-powered thermo-chemical water-splitting pathways.

Acknowledgements

The author of this research greatly appreciates the reviews and constructive comments provided by several experts in sustainability and LCA from the University of Oxford in the UK and from Harvard University in the USA. The literature materials used in this research were made available through the Bodleian Libraries of University of Oxford and Tate library at Harris Manchester College (HMC) in Oxford during this author’s tenure as a Technical Fellow at HMC in the UK.

Conflict of Interest

None declared.

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