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Life cycle assessment of hydrogen fuel production processes

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Abstract

The use of hydrogen as an alternative fuel is gaining more and more acceptance as the environmental impact of hydrocarbons becomes more evident. A life cycle assessment study has been carried out to investigate the environmental aspects of hydrogen production. Production by natural gas steam reforming and production upon renewable energy sources are examined. Hydrogen is selected as a future alternative fuel because of the absence of CO_2 emissions from its use, its high-energy content and its combustion kinetics. A very large number of environmental burdens result from the operation of the different hydrogen production routes. A complete and accurate identification and quantification of the environmental emissions has been attempted. The use of wind, hydropower and solar thermal energy for the production of hydrogen are the most environmental benign methods. The benefits and the drawbacks of the competing hydrogen production systems are presented.

Keywords: Alternative fuel; Hydrogen; Life cycle assessment; Sustainable development

1. Introduction

Hydrogen is anticipated to join electricity as the foundation for a globally sustainable energy system using renewable energy. Hydrogen can be produced safely, is environmentally friendly, and versatile, and has many potential energy uses, including powering non-polluting vehicles, heating homes and offices, and fueling aircraft.

Hydrogen is the lightest and most abundant element in the universe. The element is very reactive chemically and occurs as a free element only in trace amounts. It is found in water (H_2O), fossil fuels and all plants and animals.

Hydrogen gas (H_2) is not a primary fuel in the same sense as natural gas, oil, and coal. No wells produce hydrogen gas from geologically identified deposits. Rather, hydrogen is an energy carrier, like electricity. Hydrogen is a secondary form of energy, produced using other primary energy sources, such as natural gas, coal, or solar technologies. More than 8 million tons of hydrogen are consumed in the United States each year, primarily by the chemical and petroleum industries. While use of hydrogen in space shuttle missions is today the only significant fuel application, this use represents only about 0.1% of the hydrogen consumed. Most of the hydrogen (97%) is made by steam reforming of natural gas (which is mainly methane, CH_4) and other fossil fuels (Fig. 1). Production of hydrogen from water—either through electrolysis or direct photochemical reactions—is the most likely long-term source [1].

When hydrogen burns, it releases energy as heat and produces water

$$2H_2 + O_2 \rightarrow 2H_2O.$$

No carbon is involved, so using hydrogen produced from renewable or nuclear energy as an energy resource would eliminate carbon monoxide and CO_2 emissions and reduce greenhouse warming. Direct burning of hydrogen may still produce small amounts of nitrogen oxides, however.

The main goal of this study is a comprehensive life cycle assessment (LCA) of hydrogen production processes. LCA is a systematic analytical method that helps identify and

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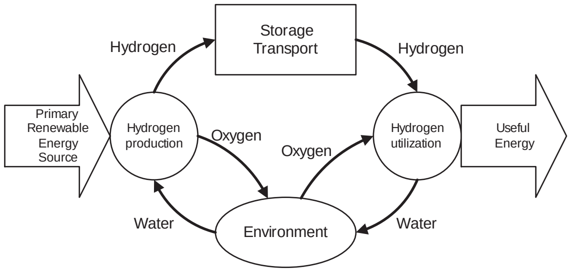

Fig. 1. The life cycle of hydrogen from RES.

evaluate the environmental impacts of a specific process or competing processes. For each process within the life cycle, detailed inventories of the material inputs and outputs are produced [2,3]. In this way, a life cycle inventory (LCI) is created which accounts for the total inputs and outputs of all flows attributable to the production of hydrogen.

The functional unit used for this work and on which all the calculations are based is 1 MJ energy produced from hydrogen. This functional unit has been chosen in order to make comparisons easier. It is important to know that 1 kg of hydrogen has a high heating value (HHV) of 142 MJ. The environmental effects of hydrogen production by natural gas steam reforming, which is today the main path of production, will be compared with the environmental effects of different production chains by the use of renewable energy sources. Ultimately, the environmental benefits and drawbacks of the competing systems will be presented [4].

The fuel systems (production and use) that are studied are the following:

A. Fuels produced from conventional sources:
   1. Hydrogen produced from steam reforming of natural gas.

B. Hydrogen produced from renewable energy sources:
   2. From solar energy using photovoltaics for direct conversion.
   3. From solar thermal energy.
   4. From wind power.
   5. From hydro power.
   6. From biomass.

2. Life cycle assessment

LCA is a powerful tool, often used as an aid to decision making in industry and for public policy. LCA forms the foundation of the newly invented field of industrial ecology [5,6]. There are several possible uses and users for this tool. It can be used to evaluate the impacts from a process or from production and use of a product. Impacts from competing products or processes can be compared to help manufacturers or consumers choose among options, including foregoing the service the product or process would have provided because the impacts are too great. In addition, LCA can identify key process steps and, most important, key areas where process changes could significantly reduce impacts. Analysts can use results to help characterize the ramifications of possible policy options or technological changes.

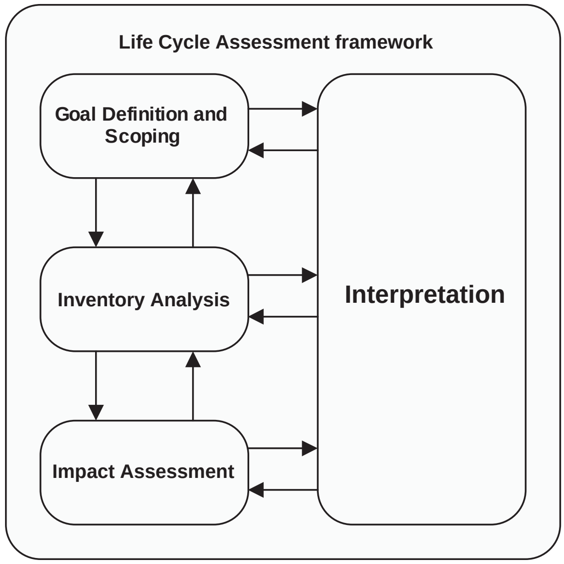

Fig. 2. The LCA framework.

The LCA process is a systematic, phased approach and consists of four components: goal definition and scoping, inventory analysis, impact assessment, and interpretation (Fig. 2). *Goal Definition and Scoping* defines and describes the product, process or activity. It establishes the context in which the assessment is to be made and identifies the boundaries and environmental effects to be reviewed for the assessment. *Inventory Analysis* identifies and quantifies energy, water and materials usage and environmental releases (e.g., air emissions, solid waste disposal, wastewater discharge). *Impact Assessment* assesses the human and ecological effects of energy, water, and material usage and the environmental releases identified in the inventory analysis. *Interpretation* evaluates the results of the inventory analysis and impact assessment to select the preferred product, process or service with a clear understanding of the uncertainty and the assumptions used to generate the results.

The entire system is examined in order to evaluate the impacts and choose the best option. The system must be defined so that the entire lifecycle is included, or important effects may be neglected. The procedures for performing the inventory part of an LCA have been very well defined by such groups as the Society of Environmental Toxicology and Chemistry (SETAC) and the International Organization for Standardization (ISO) [2,7]. Adherence to the standard methodology makes it easier for anyone to do such an analysis. The items in the standard inventory are generally energy and materials, including effluents, but lifecycle costs

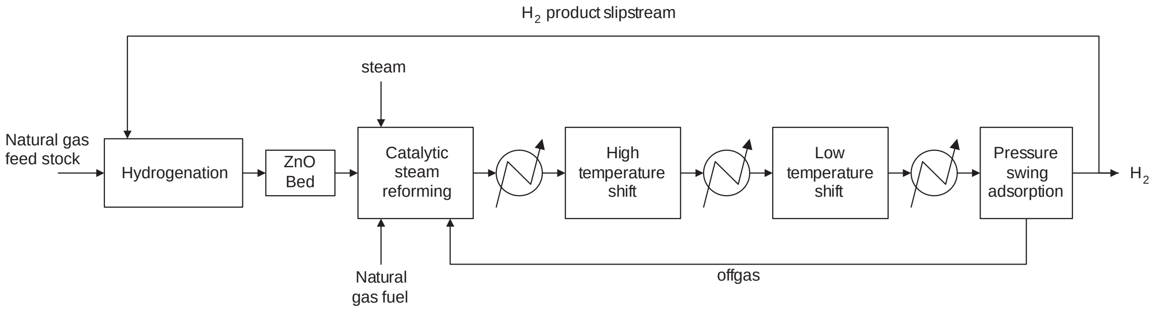

Fig. 3. Hydrogen plant block flow diagram.

can also be determined. Once data are assembled, the inventory items are added up to provide a total profile for each option. In some LCAs, the inventory is the final product. However, even though it is difficult to do an impact analysis (the final step in the LCA methodology), the inventory can provide useful information to aid decision makers.

3. Hydrogen production by natural gas steam reforming

Steam reforming is at present (and very likely will be in the future) one of the most important and most economic way of hydrogen production. In this context, it is of crucial importance that steam reforming induces the least CO_2 emission of all industrial scale processes available at present.

During steam reforming hydrocarbons are catalytically split in the presence of steam at temperatures of 800–900°C (Fig. 3) [8]. Normally, the split is proceeded with nickel catalyst in gas-fired ovens. Mostly natural gas is used as feed but heavier hydrocarbons up to naphtha can also be processed. During the catalytic split the so-called syngas is produced that mainly consists of hydrogen and carbon monoxide. The basic equation is

$$C_nH_m + nH_2O \rightarrow nCO + (n + m/2)H_2.$$

Apart from this basic reaction other reactions take place where CO_2 and soot are already produced. In the following step (the so-called shift-reaction) carbon monoxide from the syngas is transferred according to the equation

$$CO + H_2O \rightarrow CO_2 + H_2$$

into carbon dioxide and hydrogen. The reaction is catalyzed using iron oxide. During the terminating purification, the hydrogen is separated from the product gas. Today, pressure swing adsorption (PSA) is the prevailing process. The remaining product gas is piped back and used as fuel to fire the steam-reforming reactor. After the fuel gas has passed several heat exchangers, it is finally released into the atmosphere.

Table 1 is a list of the major air emissions that result from the production of H_2 by natural gas steam reforming that were used for the purpose of this study [8].

Table 1
Average air emissions from H_2 production by natural gas steam reforming [8]

Air emission	System total (g/kg H_2)
Benzene (C_6H_6)	1.4
Carbon dioxide (CO_2)	10662.1
Carbon monoxide (CO)	5.9
Methane (CH_4)	146.3
Nitrogen oxides (NO_x as NO_2)	12.6
Nitrous oxide (N_2O)	0.04
Non-methane hydrocarbons (NMHCs)	26.3
Particulates	2.0
Sulphur oxides (SO_x as SO_2)	9.7

4. Hydrogen production based upon renewable energy

As stated earlier, about 97% of the worldwide hydrogen production is accomplished by steam reforming of natural gas and other fossil primary energy. However, a number of innovative production paths exist for hydrogen production based upon renewable energy and some of them have been assessed in this study by carrying out an LCA of the technological systems. The investigated process chains start with the extraction of the primary energy carrier, the transportation to the hydrogen production plant, the conversion into hydrogen and the liquefaction before the final use (Fig. 4).

The following renewable energy sources were examined:

1. Solar energy using photovoltaics for direct conversion.
2. Solar thermal energy.
3. Wind power.
4. Hydro power.
5. Biomass.

The comparative assessment of the different hydrogen production scenarios was made with the use of the Global Emission Model for Integrated Systems (GEMIS) database. GEMIS was developed by the Oto-Istitute (Istitute of Applied Ecology) in Germany [9].

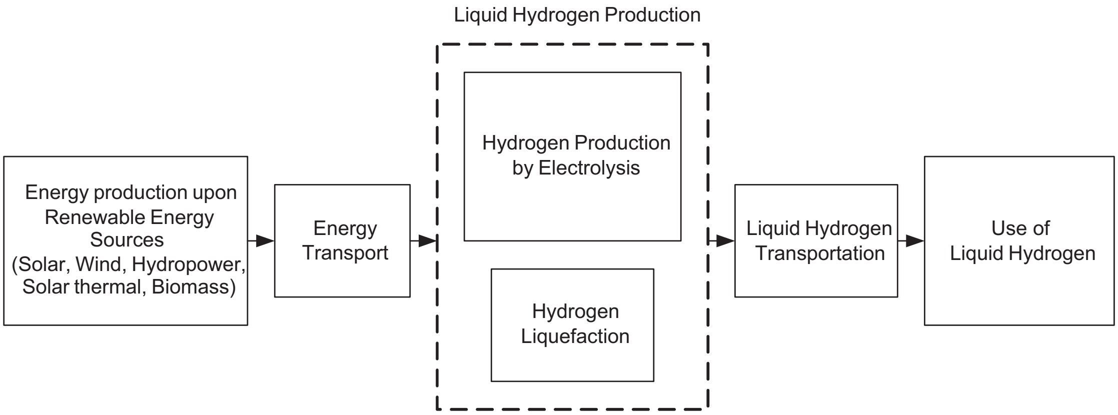

Fig. 4. Hydrogen production based upon renewable energy sources.

This study is limited to technologies for converting energy from renewable primary sources into hydrogen, thus only splitting of water is considered. From the various technologies of electrolytic hydrogen production (conventional electrolysis, (high-pressure) alkaline electrolysis, membrane electrolysis, steam electrolysis) only advanced high-pressure electrolysis is examined. This technology could be reasonable way for a future hydrogen energy production scenario [10]. Its main advantage is provision of hydrogen at high-pressure levels, which is favourable for some transport technologies; e.g., pipeline transport.

Hydrogen production by electrolysis is one of the current methods that is applied broadly and has become more mature. The overall energy efficiency of the electrolysis process is assumed to be 77% [9].

4.1. Hydrogen production by electrolysis

Electrolysis is often considered as the preferred method of hydrogen production as it is the only process that need not rely on fossil fuels. It also has high product purity, and is feasible on small and large scales.

At the heart of electrolysis is an electrolyzer, consisting of a series of cells each with a positive and negative electrode (Fig. 5). The electrodes are immersed in water that has been made electrically conductive, by adding hydrogen or hydroxyl ions, usually in the form of alkaline potassium hydroxide (KOH).

The anode (positive electrode) is typically made of nickel and copper and is coated with oxides of metals such as manganese, tungsten, and ruthenium. The anode metals allow quick pairing of atomic oxygen into oxygen pairs at the electrode surface.

The cathode (negative electrode) is typically made of nickel, coated with small quantities of platinum as a catalyst. The catalyst allows quick pairing of atomic hydrogen into pairs at the electrode surface and thereby increases the rate of hydrogen production. Without the catalyst, atomic hydrogen would build up on the electrode and block current flow.

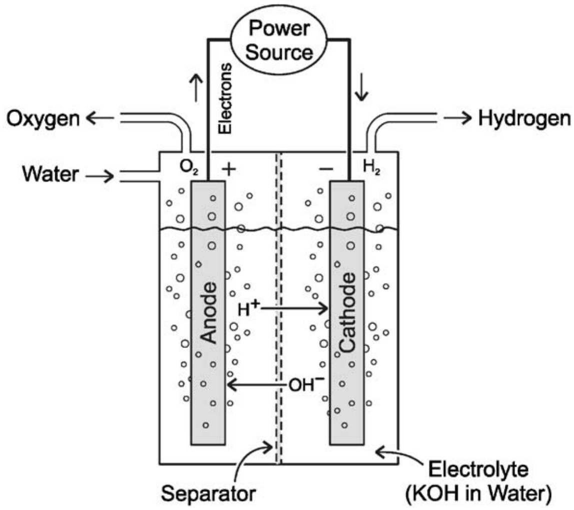

Fig. 5. Typical electrolysis cell.

A gas separator, or diaphragm, is used to prevent intermixing of the hydrogen and oxygen molecules although it allows free passage of ions.

The reaction at the cathode are:

(1) $K^+ + e^- \rightarrow K$	A positively charged potassium ion is reduced.
(2) $K + H_2O \rightarrow K^+ + H + OH^-$	The ion reacts with water to form a hydrogen atom and a hydroxyl ion.
(3) $H + H \rightarrow H_2$	The highly reactive hydrogen atom then bonds to the metal of the cathode and combines with another bound hydrogen atom to form a hydrogen molecule that leaves the cathode as a gas.

The reactions at the anode are:

(1) $OH^- \rightarrow OH + e^-$	A negatively charged hydroxyl ion is oxidized.
(2) $OH \rightarrow \frac{1}{2} H_2O + \frac{1}{2} O$	The ion reacts to form water and an oxygen atom.
(3) $O + O \rightarrow O_2$	The highly reactive oxygen atom then bonds to the metal of the anode and combines with another bound oxygen atom to form an oxygen molecule that leaves the anode as a gas.

The rate of hydrogen generation is related to the current density (the current flow divided by the electrode area, measured in ampere per meter square). In general, the higher the current density, the higher the source voltage required and the power cost per unit of hydrogen. However, higher voltages decrease the overall size of the electrolyzer and therefore result in a lower capital cost. State-of-the-art electrolyzers are reliable, have energy efficiencies of 65–80%, and operate at current densities of about 186 A/ft^2 (2000 A/m^2).

For electrolysis, the amount of electrical energy required can be somewhat offset by adding heat energy to the reaction. The minimum amount of voltage required to decompose water is 1.23 V at 77 F (25°C). At this voltage, the reaction requires heat energy from the outside to proceed. At 1.47 V (25°C) no input heat is required. At higher voltages (and same temperature), heat is released into the surroundings during water decomposition.

Operating the electrolyzer at lower voltages with added heat is advantageous, as heat energy is usually less costly than electricity, and can be recirculated within the process. Furthermore, the efficiency of the electrolysis increases with increased operating temperature. For the electrolytic hydrogen production, the thermodynamic losses are mainly due to irreversibilities associated with heat production from high-quality energy resources (fossil fuels), electricity generation and water splitting [11].

4.2. Liquefaction process

Hydrogen must be cooled down to −253°C to be liquefied. From the thermodynamic point of view, the best liquefaction process is a combination of isothermic compression followed by adiabatic expansion, whereby the gas cools down due to the Joule–Thomson effect. A quantity of 0.97 kWh/kg heat, a condensation enthalpy of 0.13 kW/kg and an energy release of 0.2 kW/kg due to the Ortho–Para-conversion has to be withdrawn for liquefaction of hydrogen. The theoretical minimum energy requirement is due to the Carnot-efficiency much higher, approximately 4 kWh/kg, depending on process management. In reality, however, none of these ideal processes is reached and therefore plants cool down the gas gradually, usually by pre-cooling it with liquid nitrogen. An electricity requirement of 0.347 MJ/MJ (0.00244MJ/kg H_2) is given in the GEMIS database (refer to 30 bar inflow pressure).

5. Comparative assessment of hydrogen fuel production

During the previous part of the study, the inventory of different fuel production processes was presented. Hydrogen production from conventional and renewable sources was thoroughly analyzed. The next step of the study is the impact assessment, to see how the specific substances affect the environment. The impact assessment evaluates the magnitude and significance of the potential environmental impacts of the different life cycles under study. It consists of three steps: classification, characterization and valuation [12]. The categories that have been examined in our study are four: global warming potential (GWP), acidification effect, eutrophication effect and winter smog effect. The reason for this is based on the nature of the data collected and the importance of these impact categories.

5.1. Greenhouse gases emissions

Although CO_2 is the most important greenhouse gas and is the largest emission from this system, quantifying the total amount of greenhouse gases produced is the key to examining the GWP of the different systems (Fig. 6). The GWP is a combination of CO_2, CH_4, and N_2O emissions. The GWP can be normalized to CO_2 equivalent emissions to describe the overall contribution to global climate change. As shown from the figure, the variation of CO_2 eq. emissions of different processes is quite large. H_2 from natural gas has by far the larger emissions.

5.2. Acidification emissions

Acidification is measured as the amount of protons released into the atmosphere. The weighting factors are presented either as mol H+ or as kg of SO_x equivalent. The two types of compound mainly involved in acidification are

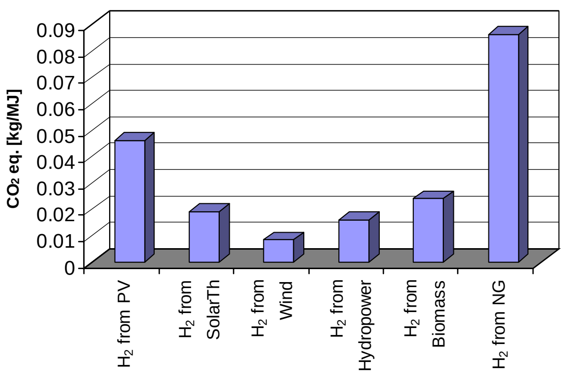

Fig. 6. CO_2 equivalent emissions from hydrogen production.

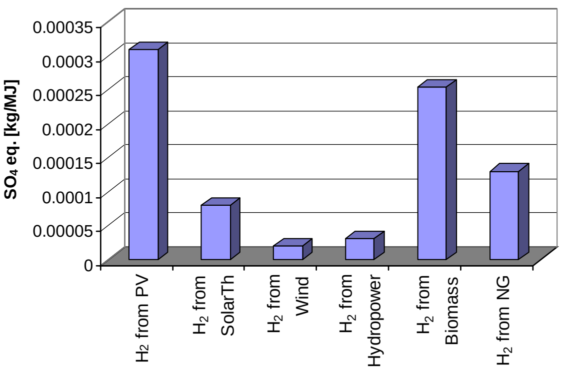

Fig. 7. SO_4 equivalent emissions during hydrogen production.

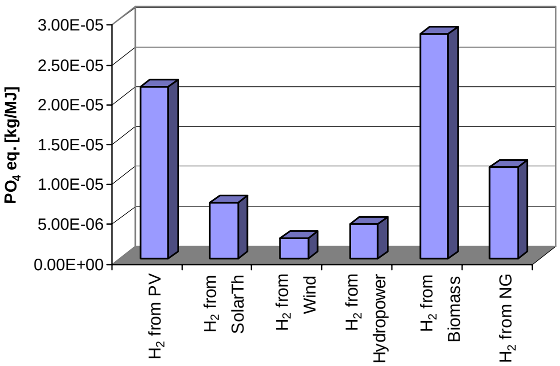

Fig. 8. PO_4 equivalent emissions of hydrogen production.

sulphur and nitrogen compounds. Chemicals like ammonia, HF, HCl, and NO_x contribute to this impact category. SO_2 and SO_x emissions are considered to have the same effect in this impact category (Fig. 7). In this category H_2 from PV has the highest SO_4 eq. emissions.

5.3. Eutrophication air emissions

Nitrogen and phosphorus are essential nutrients for the regulation of ecosystems. Enrichment (or eutrophication) of water and soil with these nutrients may cause an undesirable shift in the composition of species within the ecosystems. Eutrophication of terrestrial ecosystems is mainly due to (long distance transport of) atmospheric emissions of NO_x (nature areas) and emissions to soil of nitrogen and phosphorus (agricultural areas).

Nutriphication potentials are available for all important eutrophying compounds. It is important to note that there are available nutriphication potentials for compounds to air and to water. For the purposes of this project only the emissions which are released to air are studied (Fig. 8). H_2 from biomass has the highest value of PO_4 eq. emissions due to the fact that biomass combustion results in high NO_x emissions.

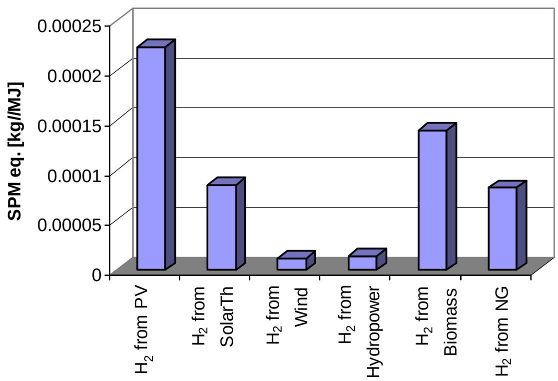

Fig. 9. SPM equivalent emissions of hydrogen production.

Table 2
Eco-indicator 95 normalization and evaluation factors [12]

Impact category	Normalization	Evaluation
Greenhouse	0.0000742	2.5
Ozone depletion	1.24	100
Acidification	0.00888	10
Eutrophication	0.0262	5
Heavy metals	17.8	5
Carcinogenics	106	10
Winter smog	0.0106	5
Summer smog	0.0507	2.5
Solid waste	0	0

5.4. Winter smog effect emissions

For evaluating winter smog, the winter smog potentials (WSP) are used for converting the different chemical emissions (dust, SO_2) to an equivalent basis. In this case, solid particulate matter (SPM) is used as the equivalent chemical compound. Fig. 9 displays the equivalent emissions of SPM during the production of hydrogen. The production of H_2 from photovoltaics is shown to have the highest SPM eq. emissions and this is due to primarily to the production stage of PVs.

6. Normalization and evaluation

Normalization is defined as an optional element relating all impact scores of a functional unit to the impact scores of a reference situation. The aim of normalization is to relate the environmental burden of a product to the burden in its surroundings.

In this study, the Eco-indicator 95 weighting method for environmental effects that damage ecosystems or human health on a European scale is used. The calculation of normalization values have been carried out using the data

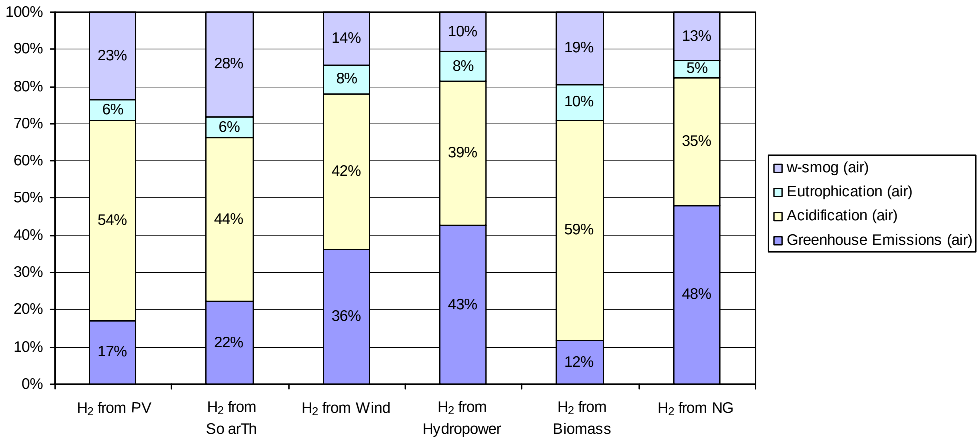

Fig. 10. Indicator graph of hydrogen production.

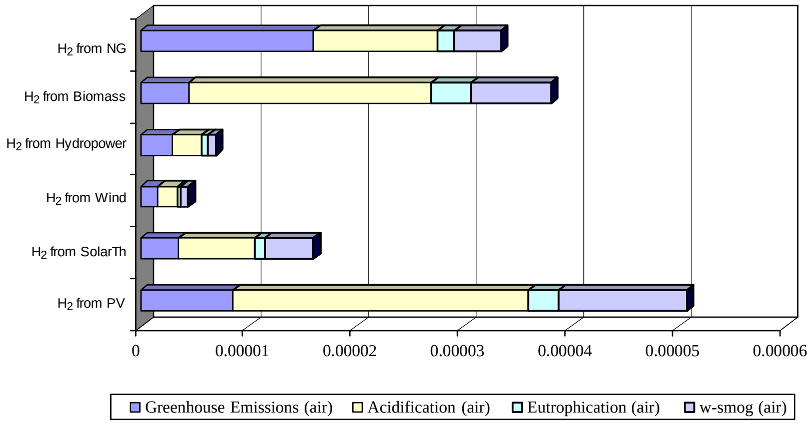

Fig. 11. Total impact scores of different hydrogen production paths.

on resource extraction and emissions, that were collected previously in a normalization study carried out for the Dutch ministry of transport and public works and the Dutch ministry of Housing, Spatial planning and the Environment (Blonk et al., 1997). These normalization values were mostly based on environmental interventions resulting from European production in 1990–1994 [12].

Normalization only reveals which effects are large and which effects are small, in relative terms. It says nothing of the relative importance of these effects. Evaluation factors are used for this purpose. Weighting factors have been applied in order to scale the seriousness of the results, measured in indicator points. The standard eco-indicators can be regarded as dimensionless figures. The absolute value of the points is not very relevant as the main purpose is to compare relative differences between hydrogen production processes. The scale is chosen in such a way that the value of one point is representative for one thousandth of the yearly environmental load of one average European inhabitant. Table 2 presents the normalization and evaluation weighting factors used for the purpose of this study.

Finally, the evaluation scores are added up to give a total impact for each material and process in the assembly. The "indicator" graph is showing the total impact scores of all the hydrogen production paths (Figs. 10 and 11).

7. Conclusions

Although hydrogen is generally considered to be a clean fuel, it is important to recognize that its method of production plays a very significant role in the level of environmental impacts. Examining the inputs and outputs from the life cycle of different production paths gives a complete picture of the environmental burdens associated with hydrogen production.

The LCA of the hydrogen systems indicates that the route of production with the use of photovoltaic energy has the worst environmental performance than all the other routes. This is attributed to the manufacturing process of the photovoltaic modules that contributes highly to all environmental impact categories of the system. At the same time the overall efficiency of the photovoltaic systems is very low. The use of renewable energy sources (RES) has the advantage of an environmentally friendly production of hydrogen, but the main disadvantage lies in their incapability to utilize a big part of the available energy [13].

High equivalent emissions of CO_2 and SO_2 have the major negative impact on hydrogen production by steam reforming of natural gas. Methane (CH_4) emissions, which primarily come from natural gas losses to the atmosphere during production and distribution, have a large effect on the GWP of the system.

The use of wind, hydropower, and solar thermal energy are proved to be the most environmentally friendly methods among the examined systems for hydrogen production. All equivalent emissions of these systems are very low.

Hydrogen derived from renewable technologies, will serve as the clean, inexhaustible energy sources in the rapidly approaching acute need for clean energy. The widespread introduction of this energy form would dramatically reduce the world's air pollution, enhance energy availability for economic development and ameliorate potential global climate problems.

The future of renewable hydrogen energy also depends strongly on reduced costs for renewable energy production. Renewable hydrogen energy will enter the marketplace when and where it is cost-effective compared to the other local forms of energy. From both an environmental and economic aspect, it is important to increase the energy efficiencies and ratios of all processes. This will lead to reduced resource consumption, emissions, waste production, and energy consumption. However, The LCA study confirms that hydrogen based upon RES offers the prospect of long-term growth in full agreement with the need to protect the environment and it will be one of the most promising energy carriers for a sustainable future.

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