Sustainability Assessment of Hydrogen Energy Pathways

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Abstract

Hydrogen is widely seen as the solution to the current problems of Global Warming and poor urban air quality. Much research and funding is being invested in the development of a "Hydrogen Economy", using hydrogen as an energy carrier for vehicles and stationary electricity production. There are a wide variety of sources for hydrogen – ranging from fossil fuels to solar electrolysis – and various options for transport and utilisation. However, the most appropriate pathway to producing and utilising hydrogen is yet to be determined, and the number of variables and uncertainty involved makes prediction difficult. This paper outlines the methodology for, and some preliminary findings of, the Life Cycle sustainability assessment of Hydrogen Energy Pathways, specifically in the Australian context. In particular, it focuses on the sustainability metrics of various hydrogen production pathways, by taking into consideration the environmental burden of pollution upon the receiving environment. This study provides an insight into the potential effects, and hydrogen production technologies that may eventually lead to a more sustainable energy pathway.

Introduction

The current environmental problems of global warming and local human health effects of pollution have been the impetus for extensive research and development of alternate energy technologies. Hydrogen is being widely examined as one potential method of reducing anthropogenic greenhouse gas (GHG) emissions, but the path to a hydrogen economy is far from certain. A variety of pathways exist for the production of hydrogen – from reformation or gasification of fossil fuels to the electrolysis of water using renewable energy sources. Many utilisation technologies also exist for both stationary and mobile applications, although most focus has been on the potential for use in fuel cells.

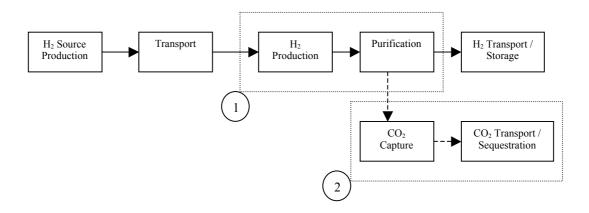
These utilisation and production pathways combine to give a large range of options for the overall life cycle, and equally large possibilities for differences in impacts. The optimum path to hydrogen, and its subsequent utilisation will vary from location to location according to local conditions of fuel availability and cost among other factors. There is a need for the establishment of a method of assessing the different options available in terms of potential and specific local impacts of the whole life cycle based on the three pillars of sustainability (social, economic, environmental).

This paper presents the concept of sustainability metrics as one possible assessment method, and gives a short example of their use.

Life Cycles for Hydrogen

This section gives a brief description of the general life cycle stages for hydrogen production and utilisation. Figure 1 shows a general representation of the main life cycle stages for the production and utilisation of hydrogen. As there are such a wide variety of feedstocks and processing methods, the combinations give a large number of pathways, all of which should be analysed to determine the most economically, socially and environmentally beneficial.

Figure 1: General Hydrogen Life Cycle



Notes: Section 1 is typically conducted within the same plant, but may be separate depending on economic and environmental factors

Carbon capture and storage is yet to be proved feasible, but should be examined as an option

Extraction

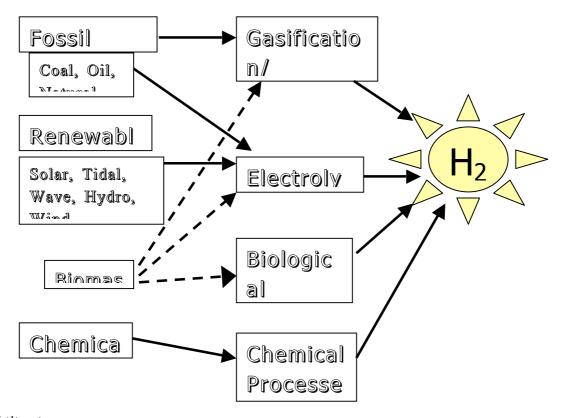
The feedstock for hydrogen production must be mined, harvested or collected to a central point for the production process. Extraction location depends on the source availability, and thus the opportunity for alternatives may be limited. The location tends to be separated by significant distance from the point of end usage, which has both advantages and disadvantages in terms of sustainability. Major impacts at the point of extraction include fugitive hydrocarbon emissions, change in land use, emissions from onsite equipment, change in amenity, local employment and consumption. The most tangible of these impacts is the impact of emissions, which may be calculated or estimated from industrial data.

Production

Hydrogen can be produced from a variety of feedstocks via various routes (see Figure 2). Currently the most common methods are Steam Reforming of natural gas (NG) and gasification of coal, typically for the ammonia and petroleum industries [1]. The production site impacts will be much the same as for extraction, although this stage has much more room for flexibility in location of the plant. Again, the focus for this

paper will be on emissions, but further work should include the less readily quantifiable categories of land use, local employment and health.

Figure 2: Hydrogen Production Pathways



Utilisation

The utilisation technology that is most commonly associated with hydrogen applications is the fuel cell. A variety of different types of fuel cells are available, each of which has different purity constraints and suitability for different applications. The high temperature Molten Carbonate and Solid Oxide fuel cells tend to be more resistant to catalyst poisoning by CO and CO₂, but are still susceptible to sulphur poisoning.

Transport

There are a number of transport stages within the overall hydrogen life cycle which need to be examined and compared in terms of the triple bottom line. Firstly, the transport of feedstock to the hydrogen production plant. Typically modern coal power stations are built at or near the site of fuel extraction, but this may not be the best method in terms of hydrogen production, as cost of transportation of hydrogen or coal, environmental and human health impacts of the plant location must be analysed and compared. Secondly, the transport of processed syngas or hydrogen from the production plant to the end usage point. Thirdly, potential transport of carbon dioxide and other by-products to storage sites.

Extensive networks of pipelines, road and rail links exist for the transport of fossil fuels for trade and domestic electricity production. Further analysis must examine

whether the production of hydrogen would be best at source or closer to the point of end use. It may be possible to use existing NG transmission pipelines to transport hydrogen or hydrogen / NG blends however, this would depend strongly on the ability of current pipeline materials to withstand hydrogen embrittlement [2], and have sufficient integrity to minimise leakage.

Existing infrastructure for the transport of feedstock would suggest that it may be most economically efficient to bring the feedstock to the processing location, which would be closer to the end user. This would eliminate some of the capital costs of hydrogen pipelines, which are around twice the cost of NG pipelines [2]. Whether this would be the most environmentally beneficial method is yet to be seen.

Storage

Storage of hydrogen is problematic due to the small size of the molecules, which make losses easy and liquefaction difficult. The main methods of storage are as a liquid or compressed gas, but metal hydrides are being examined as a chemical storage alternative. The adsorption of hydrogen onto carbon nano-materials has also been extensively researched, but is yet to prove viable. Some methods of storage will produce emissions of sorbent materials, and all will be likely to have fugitive hydrogen emissions which may have effects on ozone depletion.

Carbon Capture and Storage

For the ultimate reduction of GHG emissions, it is essential to remove CO₂. Although it is yet to be proven viable, the capture of CO₂ and storage underground in geological structures, unminable coal seams or exhausted oil and gas wells, or in the deep ocean, are some of the proposed methods. These processes cannot be relied on for the present, and will not be examined further in this paper.

Sustainability Metrics

With all the possibilities of production, utilisation, transport and carbon storage processes, there are a wide variety of pathways available for the hydrogen life cycle. The challenge then, is to assess these in terms of the sustainability of their impacts using a triple bottom line approach. This paper focuses on environmental assessment, but this approach can be extended to include the other two pillars of sustainability – the economic and social aspects.

The method of sustainability metrics has been demonstrated recently as a possible method of comparison of different process options. The Institution of Chemical Engineers (IChemE) has released a recommended procedure for measuring sustainable development progress [3]. This method is similar to life cycle analysis (LCA) methods which determine overall emissions, resource usage and economic indicators per unit of product or value added. This allows a process to be monitored for sustainability improvements, or to compare different process options, but does not include specific local parameters. This lack of specificity may reduce the potential of this technique to assess different locality options. Advances made on this technique by Diniz da Costa and Pagan [4] as followed in this paper, go some way towards

addressing this problem, but still retain some limitations due to the lack of temporal and spatial factors.

The first step in the sustainability metrics method, as mandated by IChemE, is the calculation of the environmental burden caused by a substance on the receiving environment via Equation 1, below:

Equation 1

$$EB_i = \underline{\hspace{1em}}(W_N)(PF_{i,N})$$

Where:

 EB_i = ith environmental burden

W_N = weight of substance N emitted, including accidental and unintentional emissions

 $PF_{i,N}$ = potency factor of substance N for the ith environmental burden

(IChemE and the National Pollutant Inventory have PF lists.)

The IChemE method ends here, whereas Diniz da Costa and Pagan continue by next calculating the Potential Environmental Impact (PEI). In this paper, the PEI was derived by calculating the EB and normalizing by dividing the total mass load emitted per year by the total amount of hydrogen exported per year. The PEI indicates a potential for environmental impact rather than an actual environmental impact, and is determined as follows:

Equation 2

$$PEI = \frac{\sum\limits_{i=1}^{i=n} \left(EB_1 + EB_2 + \dots + EB_n \right)}{H_{ex}}$$

Where:

PEI = Potential environmental impact for the main emission substances Hex = Total hydrogen exported (GJ)

Diniz da Costa and Pagan [4] indicate that the PEI can be viewed as a technology indicator, as it gives an overall assessment of the performance of plants relative to one another. However, it still does not take the local environment into account, thereby effectively classing all environments as the same. To overcome this, they develop Specific Environmental Impacts (SEI).

SEI indicators are developed to determine whether the emissions upon a receiving environment can cause an impact or not. If the environment has the ability to treat and buffer the emissions, then impacts are not considered significant (and may be assigned a value of 0). One example they use is that if there is no rain or if soils are alkaline, then emissions relating to acidification impacts on soil and water may not breach the carrying capacity of the local ecosystem. The approach to determine the SEI is derived from PEI as formulated below:

Equation 3

$$SEI = \underline{\quad} (SEB_1 + SEB_2 + ... + SEB_n) / H_{ex}$$

Specific Environmental Burdens (SEB) are initially derived from a linear relationship of single or multiple dimensionless average parameters as shown below:

Equation 4

$$SEB_i = EB_i(K_i)$$

Where:

K =specific environmental dose value

Equation 5

$$K = \sum_{n=1}^{n=n} \left(\frac{\frac{\alpha_1 + \alpha_2 + \dots + \alpha_n}{n}}{\left(\frac{\alpha_1 + \alpha_2 + \dots + \alpha_n}{n}\right)_{high}} \right)$$

Where:

_ = dimensionless parameter n = number of parameters

This approach provides a set of values normalized using the highest value of K of the plants being examined (or a base case plant). This solves the problem that arises when (as is typical with environmental parameters), there are values varying over several orders of magnitude.

To use specific sustainability indicators, it is necessary to have data relating to the specific location of a plant or process. Where an impact is global in nature (such as emissions of greenhouse gases), the specific impact may be assumed to be equal to the potential impact.

Test Case

An example of the use of this method is described here, using the production of 67.85 t H_2 / d or 9581 GJ/d (the equivalent to provide fuel for 5000 fuel cell buses and 100,000 fuel cell cars, based on the average Australian driving patterns and the work of Ogden, et al. [5]). The two cases compared are production using NG or coal at the point of production for theoretical supply to Brisbane. Only extraction, source transport and hydrogen production emissions are considered here, due to the limits of time and data availability.

Table 1: Hypothetical Test Case Data

Feedstock	Coal	Coal	NG	NG
Process	Gasification	Gasification	Steam	Steam
	(IGCC)	(IGCC)	Reforming	Reforming
Location	#1	#2	#3	#4
Distance from	Onsite	200km	Onsite (3km)	450km
Source	(3km)			
Transport Type	Rail	Rail	Pipeline	Pipeline
Mean Annual	92	66	95	53
Days of Rain				
Average soil pH	5.8	7.3	5.7	6.4
Population within	1075	274955	812	5749
20km				

Transport distances in this case are based on typical distances from operating gas fields / coal mines to major centres [6]. Overall emissions due to transport were calculated using estimates of per tonne kilometre emissions based on a recent European study by Edwards, et al. [7] and Queensland Rail's report on road / rail emissions [8]. The emissions data that was utilised in the sustainability metrics was calculated using literature average values. Some emissions were not available due to commercial confidentiality, but estimates will be made during further work.

In the case of Global Warming Potential, the function $f(_)$ giving the specific environmental dose value, K, is assumed equal to the PEI, as global warming is a world wide issue, so the specific impact of emissions is equivalent to the potential impact. For Acidification, $f(_)$ is given as the average of two factors – one relating to mean annual days of rain and the other to soil pH. But where there is no rain, or the soil is alkaline (and thus may have the ability to buffer the effects of acid rain), the K value is 0.

Rain factor:

Equation 6

$$_{\rm rain} = f_{\rm rain} / 365$$

Where f_{rain} is the mean annual days of rain.

Soil factor:

Equation 7

$$\alpha_{soil} = \left(1 - \frac{pH_{soil}}{pH7}\right)$$

According to the IChemE [3] NO_x may be given a weighting of 0.7 as compared to SO_x (as SO_2) which are given a weighting of 1. The combined sum of these weighted emissions is then multiplied by the K value to give the specific impact.

The factor for human health effects of particles less than 10µm in size (PM₁₀) depends on population within certain distances of the plant. Particulate matter tends to settle

within 20km of the emission point, For the purposes of this study, it has been estimated that the impact of PM_{10} is focussed within the first 20km of a plant, with the population outside that radius receiving only minimal impact.

Equation 8
$$f(__{pop}) = P_{20km}$$

where P_{20km} is the population within a 20km radius.

Results

Three major impacts were analysed in the test case – Global Warming, Atmospheric Acidification and Human Health effects of small particles. Analysis was completed on each individual stage of the life-cycle, however it is possible to make the comparison between stages depending on the desired outcome. The effect of using the specific environmental impact approach is to reduce the effect of the smaller impacts further – thus spreading the values over a wider range. This implies that the higher emitters of CO_2 per GJ H_2 are penalised further in terms of the measure of their sustainability, whilst the lower emitters have enhanced performance.

Figures 3 and 4 show the outcome of the global warming impact resultant from CO₂ emissions related to hydrogen production and transportation components. It is observed that large impacts are allocated to production while transportation results in impacts of two order magnitude lower.

Figure 3: H2 Production Impacts on Global Warming

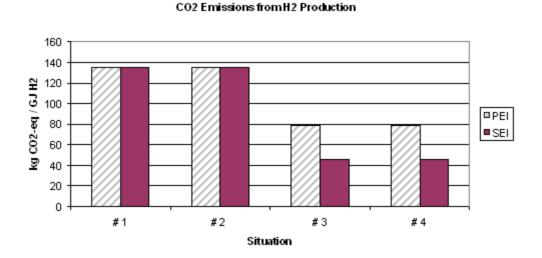
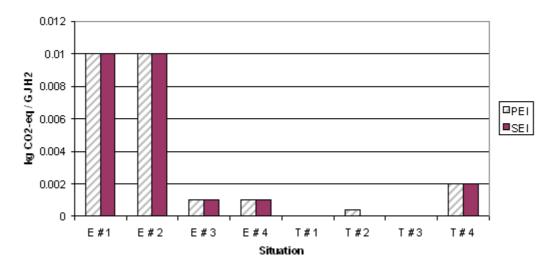


Figure 4: Impacts of Feedstock Transport and Extraction Emissions on Global Warming

Extraction (E) and Feedstock Transport (T) CO2 Emissions



Acidification impacts take into account the local soil and weather conditions and the results are depicted in Figures 5 and 6. It is assumed that where there is soil of pH greater than 7, the environment has some capacity to buffer the impact of acid compounds, and thus no impact is recorded. Thus the only impact that is unusual is situation #2, which is lower than all others due to high soil pH. This is perhaps the best example of where the specific sustainability impact is important, as it brings local conditions into account.

Figure 5: Impacts of Hydrogen Production Emissions on Atmospheric Acidification

Acidification Impact of H2 Production

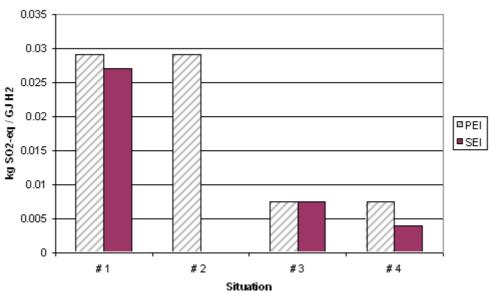
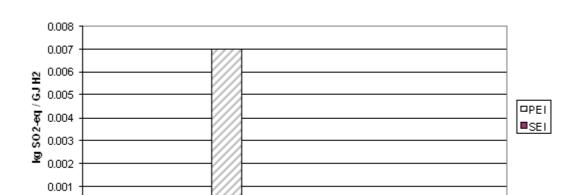


Figure 6: Impact of Feedstock Transport Emissions on Atmospheric Acidification



Feedstock Transport Acidification Impacts

Figure 7 shows the impact of PM_{10} emissions on human heath. The impact of particulates was expected to be high in areas of higher population density, and it proved to be so. The important point here is the comparison of situation #1 and #4. Typically it would be expected that a natural gas plant would be better than IGCC, but due to population density, it would actually have less of a health impact to build plant #1 rather than plant #4.

Situation

#3

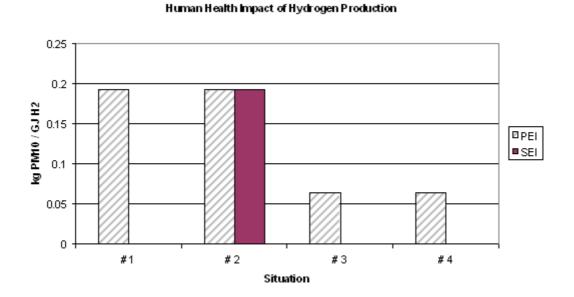
#4

Figure 7: Impact of Hydrogen Production PM₁₀ Emissions on Human Health

#2

O

#1



Tables 2 and 3 summarize the sustainability metric results for the hydrogen production and transportation components for the considered impacts in this study: global warming, acidification and human health. Global warming far exceeds the other impacts by four to five orders of magnitude.

Table 2: Summary of Results - Hydrogen Production Impacts

	Global Warming		Acidification		Human Health	
Situation	PEI	SEI	PEI	SEI	PEI	SEI
#1	135.3	135.3	0.0291	0.027	0.1925	0.0008
#2	135.3	135.3	0.0291	0	0.1925	0.1925
#3	78.5	45.6	0.0075	0.0075	0.064	0.0002
#4	78.5	45.6	0.0075	0.0039	0.064	0.001

Table 3: Summary of Results - Feedstock Transport and Extraction Impacts

Transport	Global Warming		Acidification	
Situation	PEI	SEI	PEI	SEI
#1	$5x10^{-6}$	1x10 ⁻⁸	0.0001	0.00009
#2	0.0004	$7x10^{-5}$	0.007	0
#3	0.00002	2x10 ⁻⁷	6x10 ⁻⁷	6x10 ⁻⁷
#4	0.002	0.002	0.00004	0.00002

Extraction	Global Warming		
Situation	PEI	SEI	
#1	0.01	0.01	
#2	0.01	0.01	
#3	0.001	0.0001	
#4	0.001	0.0001	

In order to demonstrate the use of sustainability metrics in terms of comparing different life cycle stage impacts, Table 4 shows the results of such an analysis.

Table 4: Specific Environmental Impacts for Global Warming - Comparison of LC stages

	Extraction	Transport	Production
#1	6.95E-07	1.85E-13	135.3
#2	6.95E-07	1.18E-09	135.3
#3	2.15E-08	5.09E-12	78.53
#4	2.15E-08	6.74E-08	78.53

Discussion

As mentioned briefly above, the results were in line with expectations in the majority of cases. Due to the assumption here that the climatic conditions were approximately equal across the entire life cycle regardless of distance, the SEI becomes the PEI for the comparison of different life-cycle stages apart from Global Warming Impacts, which are shown in Table 4. It is apparent that the impact of transport emissions tends to be the least, except for long distance natural gas pipelines, where the impacts overtake extraction emissions. The global warming impacts are as expected, with longer distance transport, coal extraction and IGCC having higher impacts. Large differences in order of magnitude are observed due to the method utilised, which extends the difference between low and high emissions. This may be useful in encouraging the lowering of emissions, but can also be misleading at first glance, as it shows a much lower impact on Global Warming than actually exists. It may be more appropriate to leave the K factor as 1 in this case, as PEI can be assumed equal to the SEI with such a global-scaled impact.

The Atmospheric Acidification and Human Health impacts give a good indication of the amount of data required to utilise these sustainability metrics. Data such as average rainfall for specific areas, average soil pH and local population within certain distances of the emissions source can be expensive to acquire - both in monetary and time costs. Complicating matters is the distance over which the life cycle stages are spread, which may not allow the assumption of constant conditions to be justified. The method of assuming specific impacts to be zero where soil is alkaline or there is no rainfall, raises the possibility of a more highly emitting plant being ranked as more sustainable than a lower emitting plant depending on local conditions. This is shown in the test case, where the SEI of situation #2 was less than all other situations, in contrast to the PEI that was higher than most. Ultimately there must be some impact from any emission, but it is reasonable to assume that the buffering capacity of alkaline soil could lessen the impact significantly.

It is apparent that there are a number of aspects of this methodology that can be improved. The functions $f(\alpha)$ could be examined and refined further in the light of environmental data. Also, although this method attempts to include local environments, it does not include temporal or spatial factors, hence allowing only a general "whole-of-air-shed" approach.

One of the major challenges in utilising this method is the possibility of having the life cycle stages spread out over a large distance, thus allowing for great variability in local conditions, and requiring further calculations. For instance, the emissions of particulates from transport were not included here, as the data requirements would require section by section (kilometre by kilometre or point by point) analysis. This means that it makes little sense to add the total life cycle emissions prior to analysis, unless it can be reasonably assumed that the conditions are constant throughout the area analysed – a dubious assumption in the case of human health and acidification effects. Also, some emissions are not included or the location cannot be specified, for example the NOx and SOx emissions from offsite electricity production.

This approach is a comparative method, which can be used variously to assess the impact of different technologies, locations or performance of a plant over time. By comparing different technologies, we may find the best option for a certain location, or alternately we can try to find the best location for a technology to have the least impact. We could also monitor a plant on a regular basis to determine whether it is being made more or less sustainable. The approach taken here has been to compare the different options among themselves, however it may be preferred to compare to either an ideal or a worst acceptable case example. Or alternatively, comparison could be based on current or projected legislative requirements for power generation emissions. This would offer the benefit of a universal yardstick, but could be practically very difficult to derive and implement in order to take the specific local impacts into account.

The measurement of a baseline for environmental factors (from which a deviation can be measured) is often difficult due to diurnal and seasonal variations, and the fact that most environments have already been affected by human activity. Also, estimating the assimilative capacity of the environment could be exceptionally difficult, as the effects of incremental changes in ambient levels of emissions may not be obvious. Ultimately, the goal of zero emissions could be the benchmark for improvement of a plant, but it does not give an indication of whether a non-zero emissions plant is sustainable or not.

The great advantage of this method is the inclusion of local factors, which can change the level of impacts significantly. This should allow a more reasonable estimate of sustainability.

Conclusions

This work shows an initial application of sustainability metrics to the life cycle of hydrogen which has been demonstrated in a test case. The method utilised has many areas that merit further development, in particular to take into account temporal and spatial variations of emissions over air sheds. The results show that global warming will continue to be a major issue of environmental concern for a hydrogen economy reliant on fossil fuels. Although it is expected that much lower emissions will be produced at the user end (i.e. fuel cell cars), CO2 emissions from hydrogen production exceed by several order magnitudes acidification and human health impacts. The global warming impacts are higher with longer distance transport, coal extraction and IGCC. Large differences in order of magnitude are observed due to the method utilised, which extends the difference between low and high emissions. This may be useful in encouraging the lowering of emissions, but can also be misleading at first glance, as it shows a much lower impact on Global Warming than actually exists.

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