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Real world renewable hydrogen transport.

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Real World Renewable Hydrogen Transport

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Abstract: Hydrogen represents an excellent energy storage option as it can act as both a short and long-term energy store. As the UK Government is strategically moving the UK towards a low carbon economy, hydrogen can play an important role as a solution to make use of grid constrained 'green' energy in transport.

In the transport sector, green hydrogen produced from renewable sources offers one of the best opportunities to reduce green house gas emissions and significantly reduce dependence on fossil fuels. Use of zero carbon or 'green' hydrogen derived from renewable sources in Fuel Cell Electric Vehicles (FCEV) is expected to lead to a 90%- 95% reduction in well-to-wheel emissions by 2020 when compared to existing internal combustion engines [1].

Described within this paper is a real-world case study that utilises grid constrained renewable energy (instead of discarding it) as a source of clean energy to produce 'green' hydrogen for use in a transport application. A model that simulates hydrogen demand from transport has been developed. A Simulink model of hydrogen production, storage and cascade refuelling operations has also been presented. The modelling of a real world application of hydrogen transport technology demonstrates how an electrolyser could be sized to provide the daily hydrogen fuel demand for a real-world commercial hydrogen transport application.

Keywords: Hydrogen, renewables, zero carbon fuel, energy storage.

INTRODUCTION

Hydrogen is considered an energy vector rather than an energy source. When hydrogen is generated from zero carbon energy sources it can provide storage for provision of zero carbon on-demand electricity as well as long-term option for decarbonising road transport. Currently there are relatively few hydrogen vehicles in operation. It has been estimated that cumulative worldwide shipments of fuel cell vehicles from 1997-2009 were of the order of 1,000 vehicles [2]. However recent market analysis concludes that a pre-commercialisation period began in 2010 and is predicted to continue through to 2014. During this period, it is expected that up-to 10,000 hydrogen FCEV will be deployed [3]. From 2015, forecasts suggest 57,000 FCEVs will be sold annually with sales volume progressively increasing to 390,000 vehicles by 2020.

In order to build real-world experience in anticipation of the eventual roll-out of hydrogen vehicles a number of trials are taking place worldwide of fuel cell passenger cars and buses. There is limited trial activity with hydrogen-fuelled commercial vehicles, despite it being widely acknowledged that 'return-to-base' commercial fleets potentially offer the most promising market for the early adoption of alternatively-fuelled vehicles. A good example of such hydrogen transport project leading to early FC vehicles commercialisation that combines both renewable energy and hydrogen energy storage technologies for the transport sector is the Scottish hydrogen bus project [4].

A recent automotive council's low carbon commercial vehicle and off-highway roadmap examined the suitability of current and emerging technologies including hydrogen to the decarbonisation of the non-passenger vehicle fleet. The study concluded that Internal Combustion Engine (ICE) vehicles fuelled by sustainable gaseous or liquid fuels will remain the most appropriate for heavy duty use [5]. One example of a 'green' gaseous fuel for use in an ICE is Hydrogen (H_2) produced from renewable energy. H_2ICE vehicles have an advantage over FCEV in that they do not require as high a purity of hydrogen as is currently needed for operation of Proton Exchange Membrane fuel cells (PEMFC). A significant barrier to the wide spread adoption of hydrogen fuelled vehicles is access to refuelling infrastructure. Described within this paper is a real world case study of a hydrogen refuelling station along with a model developed to simulate its suitability for use in refuelling a delivery vehicle application.

CASE STUDY REVIEW AND HYDROGEN DEMAND CALCULATION

The hydrogen demand in this case study is based on the characteristics of the converted petrol-hydrogen bi-fuelled Ford Transit supplied as a technology

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Table 1: Manufacturer's Vehicle Details

Parameter	Value
Model year	2009
Fuel	Petrol / compressed hydrogen (350bar)
Fuel capacity	Petrol: 80litre. Hydrogen: three tanks (2x74litre, 1x39litre) totally 4.5kg at 350bar (Low pressure alarm/warning occurs at 20 bar)
Engine	2.3 litre displacement capacity with spark ignition
Engine Cylinders	Straight 4
Engine Power	104kW (petrol); 75kW (estimated, hydrogen)
Supercharger	Belt-driven with intercooler provides additional combustion air when running on hydrogen gas
Vehicle range (un-laden)	Urban - 82 miles; Motorway - 135 miles (estimated)

demonstrator [6]. The case study hydrogen vehicle utilises 350 bar on-board hydrogen storage tanks that are similar to many other demonstration vehicles [7, 8] making the findings particularly relevant. The case study vehicle details are given in Table **1** [6]:

The total on-board hydrogen capacity is 4.52kg H_2 at 350bar and 15°C. Due to the low pressure safety alarm the transient on-board capacity is considered as 4.2kg H_2. This is based on the "low pressure" alarm occurring at 20bar with the expectation that the vehicle will be switched to petrol operation at this point. 20bar equates to 6% (20/350) of the full capacity of 350bar, therefore 6% of 4.52kg of H2 is found to be 4.2kg H_2.

The vehicles range has been reported to be between 80 – 85 miles (130 – 160km) on one re-fill. It is assumed that the vehicle will start its journey with a full tank at 350bar and stop at the "low pressure" alarm of 20 bars. Hydrogen consumption can therefore be considered as 19-20 miles/kg (given the range 80–85 miles/4.2kg), or 31-38km/kg (130–160km/4.2kg).

The vehicle is operated up to a maximum of 6 days a week (Monday to Saturday inclusive) covering close to the maximum range reported by the vehicle manufacturer every day. Therefore, it is reasonable to consider that the vehicle will require a full refill of hydrogen each day.

As the vehicle can only consume a maximum of 4.2kg due to the presence of the 'low pressure' alarm safety feature, the weekly demand for hydrogen can be calculated as 4.2 x 6 = 25.2kg. Whilst there is no demand for hydrogen on the 7th day (Sunday), it is possible for the refuelling infrastructure to be replenishing in this time.

CASE-STUDY GREEN HYDROGEN PRODUCTION

'Green' Biogas is produced at Comhairle nan Eilean Siar (CnES)'s Integrated Waste Management Facility (IWMF) from the anaerobic digestion of municipal organic waste. The rate of production varies depending on the composition and quantities of organic waste fed into the anaerobic digester.

The biogas is fed to a 240kWe gas engine producing electricity and heat which are partially re-used to supply the IWMF's energy demands. Excess electricity (where allowed) is exported to the electricity distribution network or used to provide power for hydrogen production and storage. The variable biogas production rate results in the gas engine operating periodically for between six and ten hours per day.

When the biogas engine is operating, the Hebridean Hydrogen Seed (H2SEED) facility [9] uses the excess electricity to power a 5.33Nm^3/hr or 0.46kg/hr alkaline electrolyser at Standard Temperature and Pressure to generate hydrogen for typically 10 hours per day.

MASS TRANSFER MODEL

A mass transfer model has been developed to simulate the storage and refuelling performance of the hydrogen system. The model allows the pressure, volume and stored hydrogen mass to be simulated in order to identify if it is possible for a known hydrogen demand to be met from a renewable hydrogen source.

Modelling Storage

The ideal gas relationship shown in equation 1 is used to describe the behaviour of real gases at pressures up to approximately 1450 psig (100 bars) at normal ambient temperatures [10]. However at higher pressures the results become increasingly inaccurate. Where P is pressure, ρ is the amount of mass in a given volume (m/V), R is the specific gas constant for hydrogen of 4124.18 Nm/kg K, and T is temperature in ^{o}K

$$P = \rho RT \quad (1)$$

This resulting deviation from the ideal gas law is always in the form of compression as the gas occupies less space than the ideal gas law predicts. To correct this in the model developed, a compressibility factor *Z* is utilized.

Compressibility factors (or "Z factors") are derived from data obtained through experimentation and depend on temperature, pressure and the nature of the gas. The *Z* factor is then used as a multiplier to adjust the ideal gas law to fit actual gas behaviour as follows:

$$P = Z\rho RT \quad (2)$$

The National Institute for Standards and Technology (NIST) developed a mathematical method for calculating compressibility factors using a virial equation based on Pressure and Temperature. Applying this mathematical method [11], a Simulink model has been developed providing correction factors with an accuracy of 0.01%.

Using equation 3 and the variable values listed in Table **2** [11], the compressibility factor for hydrogen at different pressures and temperatures can be easily calculated to high degree of accuracy.

$$Z(P,T) = \frac{p}{\rho RT} = 1 + \sum_{i=1}^{9} \alpha_i \left(\frac{100}{T}\right)^{bi} \left(\frac{p}{1}\right)^{c_i} \quad (3)$$

Where, P: is pressure in Mega-Pascal (MPa) and T: is temperature in Kelvin (K)

Where: The mass of diatomic hydrogen and the molar gas constant given in Table **2** are from the recent publications of this information [12, 13]. The molar mass is given to aid in conversions from molar to mass density.

The hydrogen produced from the electrolyser passes directly to a low-pressure (LP) buffer storage at up to 12bar prior to compression to the high pressure (HP) storage at up to 420 bar pressure. The LP buffer storage consists of two manifold cylinder pack (MCP) modules providing a nominal storage volume (geometric capacity) of 9,600 litres. At 15°C and 12bar the LP storage holds approximately 9.46kg of hydrogen calculated using equation 2 and 3. However, the transient (or usable) capacity of the LP storage is dependent on the operating set points of the hydrogen compression system. With an upper set point of 12bar and lower set point of 9bar the transient capacity provided is 2.35kg. This value is also calculated by using equations 2 and 3. The transient capacity defines the quantity of hydrogen that can be transferred from the LP buffer storage to the HP storage prior to replenishing the buffer by operating the electrolyser.

The high pressure storage consists of a total of fifteen composite cylinders each with a nominal geometric capacity of 82 Litres, providing a total nominal volume of 1,230 litres. At 15°C and 420 bar

Table 2: Table of Constants Required to Calculate Z

I	a_i	b_i	c_i
1	0.05888460	1.325	1.0
2	– 0.06136111	1.87	1.0
3	–0.002650473	2.5	2.0
4	0.002731125	2.8	2.0
5	0.001802374	2.938	2.42
6	– 0.001150707	3.14	2.63
7	0.9588528×10^{-4}	3.37	3.0
8	$-0.1109040 \times 10^{-6}$	3.75	4.0
9	0.1264403×10^{-9}	4.0	5.0

Molar Mass: M = 2.01588g/mol.
Universal Gas Constant: R=8.314472 J/(mol K).

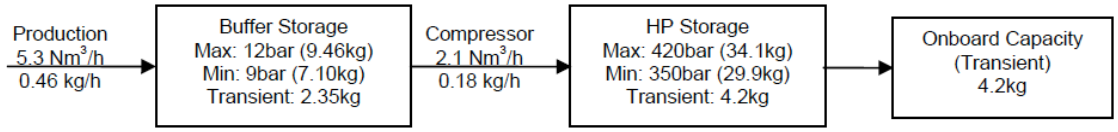

Figure1: Overview of the hydrogen system for transport application.

pressure the HP storage holds approximately 34.1kg of hydrogen using equations 2 and 3.

The refuelling station is capable of dispensing the stored hydrogen at up to 350bar in the vehicle vessels.

The hydrogen system for transport application is shown in Figure **1**.

Modelling Refuelling

The hydrogen refilling system uses a cascade fill design. In a cascade refuelling operation hydrogen held in the stationary store is transferred into the vehicle fuel tank in three stages. The three stage cascade refuelling operation is conducted in three discrete steps as follows and as shown in Figure **2** (extracted from the developed Simulink model code):

1. The first stage of a refuelling operation involves connecting a stationary 420 bar hydrogen storage tank, known as bank-1 (P_1), to the automotive storage tank (V-tank) and allowing the pressure to equalise between the two pressure vessels to give (P_2).

2. The first stage (bank-1) is disconnected from the vehicle storage tank and the second stationary 420 bar hydrogen storage tank, known as bank 2 (P_3), is then connected to the vehicle tank (V-Tank) allowing the pressure to equalise between the two pressure vessels once more.

3. The second stage (bank 2) is disconnected from the vehicle storage tank and the third 420 bar stationary hydrogen storage tank, known as bank 3, is then connected to the vehicle refuelling tank allowing the pressure to equalise between the two pressure vessels for the final time (P_4) to achieve the desired 'full' 350 bar of pressure.

Cascade Refuelling Stage 1

Using the ideal gas laws, gas constants and correction Z factors given by equations 1 to 3, the first stage of hydrogen refuelling can be expressed by equations 3 to 11 as follows:

Cascade refuelling Stage-1 Inputs

P_1 = Pressure of stationary cascade hydrogen storage bank-1

V_1 = Volume of stationary cascade hydrogen storage bank-1

T_1 = Temperature of stationary cascade hydrogen storage bank-1

R = Universal Gas Constant: R=8.314472 J/(mol K)

V_2 = (V_1) + (volume of automotive application (V-Tank))

M = Molar Mass (2.01588g/mol)

Cascade refuelling Stage-1, Z values are calculated in the Simulink model using equations 2 and 3.

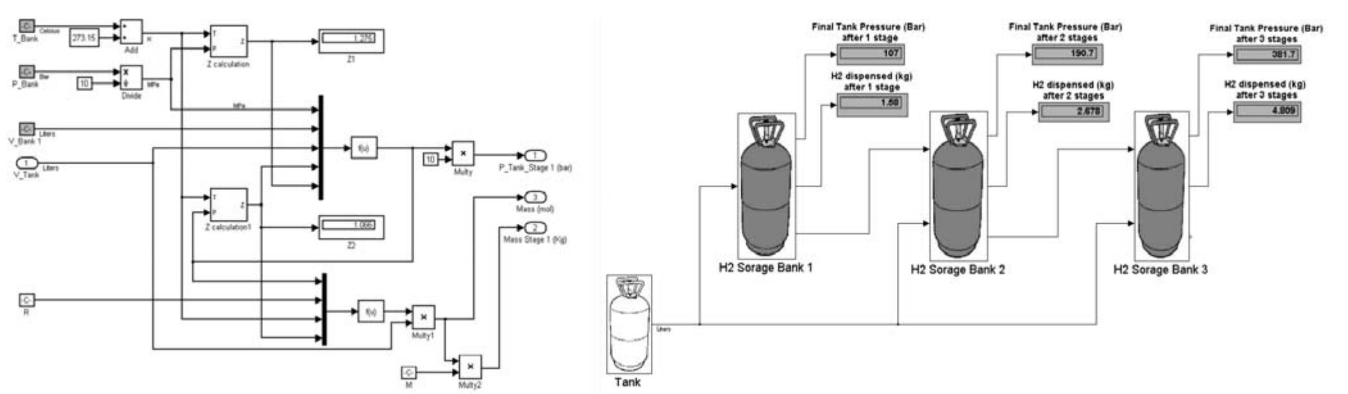

Figure 2: Simulink model code extract showing the three stage overview and stage one model.

Z_1 = correction factor for stationary cascade hydrogen storage bank-1

Z_2 = correction factor after stage-1 refuelling operation

Where:

$$P_1V_1 = Z_1 n_1 \bar{R} T \therefore n_1 = \frac{P_1V_1}{Z_1RT_1} \quad (4)$$

$$P_2V_2 = Z_2 n_2 \bar{R} T_2 \therefore n_2 = \frac{P_2V_2}{Z_2RT_2} \quad (5)$$

During the first stage of refuelling the number of moles of gas molecules present before (*n_1*) and after (*n_2*) the refuelling operation will be the same. Therefore:

$$n = n_1 = n_2 \quad (6)$$

$$\frac{P_1V_1}{Z_1RT_1} = \frac{P_2V_2}{Z_2RT_2} \quad (7)$$

When the empty vehicles hydrogen storage tank (*V-tank*) is connected to the full bank-1 hydrogen storage tank (V_1), the final cascade refuelling pressure (*P_2*) at the end of stage 1 must be calculated by solving the above equation for *P_2* as follows:

$$P_2 = \frac{P_1V_1Z_2RT_2}{Z_1RT_2V_2} \quad (8)$$

At the end of stage-1 we consider the end pressures, volumes and densities of hydrogen gas have reached equilibrium after hydrogen gas equalisation and the refuelling operation stage has completed. This means we can consider $T_1 = T_2$ and the above equation can be simplified to the following expression for P_2:

$$P_2 = \frac{P_1V_1Z_2}{Z_1V_2} \quad (9)$$

Using the values of P_2 and Z_2 and only the automotive tank volume (V-Tank) as V_2 in equation 5, it is then possible to calculate the number of hydrogen moles.

$$n_{tank} = \frac{P_2V_{tank}}{RTZ_2} \quad (10)$$

The mass (m) of the hydrogen contained within the automotive tank (V-Tank) is then found as the product of the number of moles of gas molecules present (n) and the molar mass (M) of Hydrogen.

$$m = n.M \quad (11)$$

At the end of cascade refuelling operation stage 1, the mathematical model provides:

- Final equalisation pressure and therefore pressure of automotive tank (*P_2*)
- Mass of hydrogen transferred to automotive storage tank (Kg)
- Number of moles of hydrogen (*n_{tank}*) transferred to automotive storage tank (required for calculating stage 2 refuelling operation)

Cascade Refuelling Stage-2

The stage two cascade refuelling model utilises the same equations set in stage 1, however the calculation methodology is slightly different due to the fact that the automotive hydrogen tank now contains a quantity of hydrogen.

Passed to stage-2 cascade model from stage-1 model is the number of moles of hydrogen contained within the hydrogen storage vessel in the automotive application (*n_{tank}*).

The first equation in the stage-2 model (equation 12) calculates the molar quantity of hydrogen (*n_3*) contained within the stage-2 hydrogen storage bank-2. The automotive tank already contains hydrogen at the start of stage-2 refuelling therefore $n_{tank} \neq n_3$ in this case. Therefore n_3 can be found as follows:

$$P_3V_3 = Z_3 n_3 \bar{R} T_3 \therefore n_3 = \frac{P_3V_3}{Z_3RT_3} \quad (12)$$

Where:

V_3 = volume of stationary storage bank-2

T_3 = temperature of storage bank-2

P_3 = pressure of storage bank-2

The total molar quantity of hydrogen now present when the automotive tank is attached to the hydrogen storage bank-2 can be expressed as *n_4*:

$$n_4 = n_{tank} + \frac{P_3V_3}{Z_3RT_3} \quad (13)$$

The total molar mass n_4 is therefore contained within the volume of the automotive tank (V-tank) and hydrogen storage bank-2 (V_3). Consequently the equalisation pressure (P_4) of the total molar quantity of hydrogen n_4 can now be calculated using the following equation.

$$P_4 = \frac{Z_4 n_4 R T_4}{(V_{tank} + V_3)} \quad (14)$$

With the equalisation pressure now known, along with the volume of the automotive tank (V-Tank), the corresponding molar quantity (n_5) and mass (m) of hydrogen contained within the automotive tank can be found.

At the end of cascade refuelling operation stage 2, the model provides:

1. Final equalisation pressure and therefore pressure of automotive tank (P_4)
2. Mass of hydrogen transferred to automotive storage tank (Kg)
3. Number of moles of hydrogen (n_{tank}) transferred to automotive storage tank (required for calculating stage 3 refuelling operation)

Cascade Refuelling Stage-3

The model for the final refuelling stage is similar to the stage 2 model with the molar quantity of stage 2 passed to stage 3, and the stationary value of hydrogen bank-3 used.

RESULTS OF SIMULATION

The last three rows shown in Table **3** are the results of the simulation completed on the cascade refuelling of the vehicle described in Table **1**. The first two rows of values from Table **3** are used as inputs into the cascade refuelling model to perform simulation on the cascade refuelling operation. Results shown in the bottom two rows of Table **3** indicate that the vehicle will be refuelled successfully. It can be seen that by using the cascade refuelling method that 38% of the refuelling occurs in the first stage, 26% in the second stage and 36% in the final stage.

The operating scenario described in the bulleted list below has been developed from the available hydrogen production and storage infrastructure available on the project site as described in Figure **1**. The operational hours available to run the electrolyser is also based on the renewable energy available from the bio-gas plant to produce 'green' hydrogen.

A simulation has been undertaken to identify if the vehicles daily hydrogen demand can be met by the existing hydrogen infrastructure and operational configuration. The results are shown in the last three rows of Table **3** along with Figures **3** to **5**. Based on how the hydrogen infrastructure is set up on site, the maximum daily transferable hydrogen quantity required to refuel the vehicle has been found possible to achieve from a 12 bar 5.33Nm^3 electrolyser with the hydrogen production and compression operating as follows:

- Operate electrolyser for 10 hours per day from available renewable energy
- Compress 2.03kg during the 10 hours per day of electrolyser production
- Compress 2.17kg during the following 12.8 hours
- Total transfer of 4.2kg of hydrogen into cascade refuelling station is achieved in time 22.8 hours
- Low pressure buffer pressure level at end of a 4.2Kg daily transfer becomes 9.2 bar

A Typical 7 day simulated profile of production, compression and demand are shown in Figures **3**, **4** and **5**. These have been simulated using equations 2 to 14 along with the information shown in Figure **1**, Table

Table 3: Cascade Filling Simulation Results

	Bank-1	Bank-2	Bank-3
Geometric Capacity (L)	82	82	1066
Starting pressure (Bar)	420	420	420
Pressure after refuel (Bar)	107	191	350
Mass Transferred (kg)	1.58	2.68	4.2
% of fill	38%	26%	36%

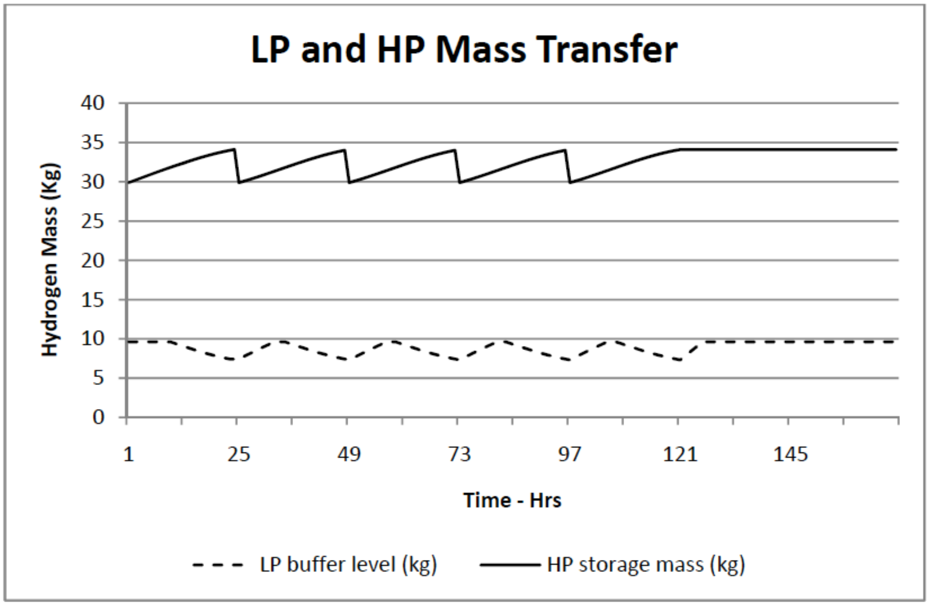

Figure 3: Hydrogen mass transfer between LP and HP storage systems.

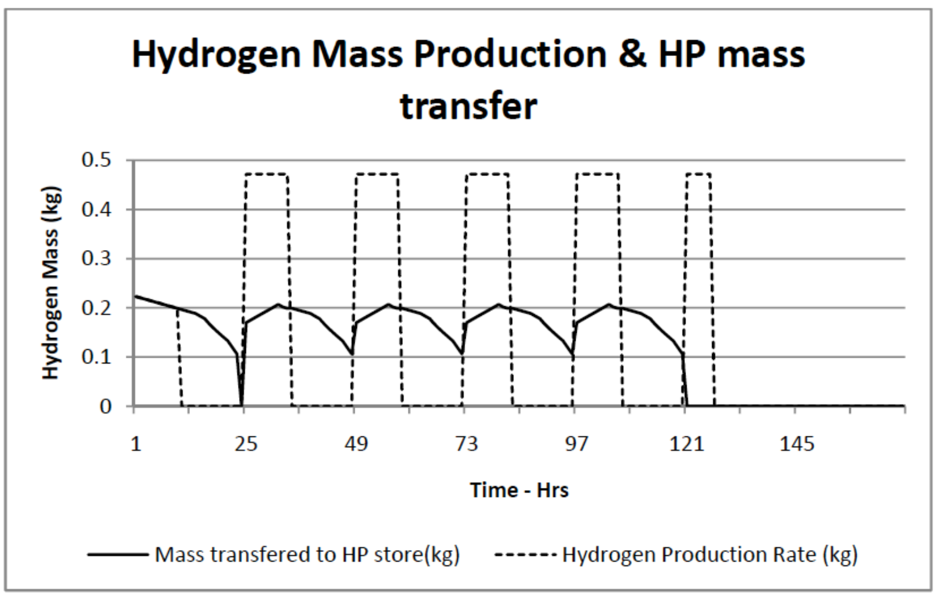

Figure 4: Hydrogen production and compression profile for 10hrs per day production.

1 and **2**. Starting condition of simulation is always assumed as full LP buffer tanks (9.62kg of H_2) and a HP storage condition after first refuelling (29.9kg H_2).

In Figure **3**, the modelling shows the HP hydrogen storage mass oscillating between 34.1kg and 29.9kg. The sudden drop in HP storage mass is attributed to the refuelling operation occurring once per day (Monday to Saturday). As the HP storage level increases, the LP storage level falls. The slow rise from 29.9kg to 34.1kg results from hydrogen being transferred from the LP buffer to the HP storage by the compressor. The slow increase in the LP buffer vessel from 7.1Kg to 9.5kg results from the generation of new green hydrogen from surplus renewable energy from the bio gas engine.

In Figure **4** the modelling shows Hydrogen mass transfer from the LP to the HP storage. The rate of transfer is given by the hydrogen compressor detailed in Figure **1**. The hydrogen production rate (restricted by available renewable energy) is also shown.

Figure **5** shows the modelling results for the HP storage pressure profile during the refuelling and replenishing periods using equations 2 and 3. This

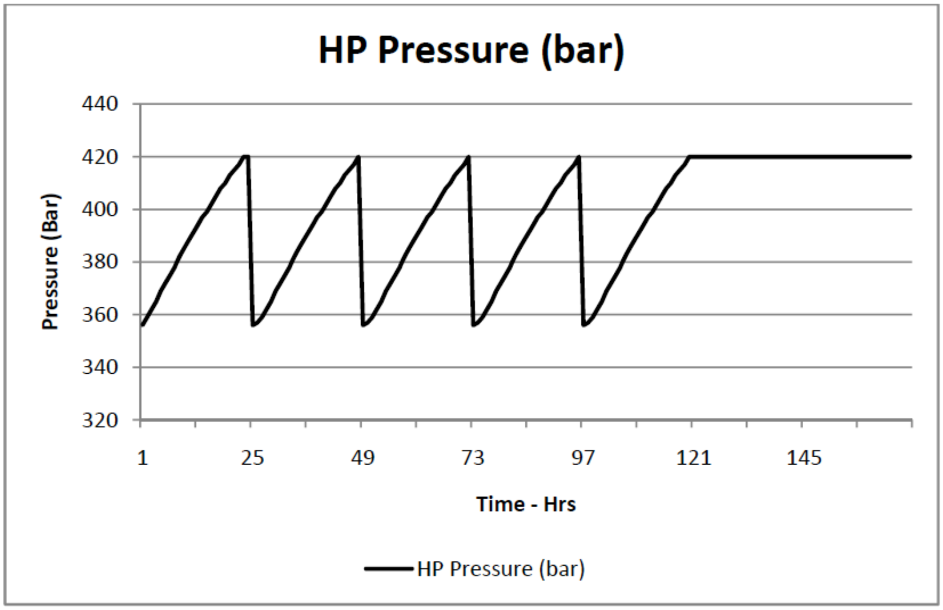

Figure 5: HP pressure cycle profile for 1 week of operation.

pressure cycling range of 350 to 420 bar shows that the refuelling operation can always achieve 350bar into the vehicle, and be replenished to 420 bar from the electrolyser and LP buffer tank.

Figures **3** and **5** together show that the vehicle will always be able to refuel to its full pressure of 350 bar, and full mass of 4.2kg. This means that the modestly sized 5.3Nm^3/h, 12 bar electrolyser powered from the available onsite renewable energy is capable of meeting the hydrogen fuel demands of the delivery vehicle with green hydrogen.

CONCLUSION

This paper has shown that a relatively small electrolyser of 5.33Nm^3/h can meet the demands of a high duty cycle commercial delivery vehicle. This is achieved by configuring the electrolyser to produce hydrogen for 10 hours per day when 'green' energy is available. The paper has proposed an infrastructure simulation for successfully fuelling a commercial vehicle activity. Simulation of the cascade refuelling configuration also showed that the vehicle can achieve a 100% fill with the configuration of cascade pressure vessels given in Table **3**.

FURTHER WORK

To enable more accurate simulation of more variable forms of renewable energy such as wind and solar power the implementation of an electrolysis production model can be added to the model.

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