INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 44 (2019) 495–510

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Techno-economic modelling and analysis of hydrogen fuelling stations

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ARTICLE INFO

Article history:
Received 28 June 2018
Received in revised form
29 October 2018
Accepted 4 November 2018
Available online 28 November 2018

Keywords:
Hydrogen refuelling station
Economic analysis
Energy costs
Setup costs
Cost-efficiency

ABSTRACT

Climate change is probably the most relevant global challenge. For this reason, governments are promoting energy efficiency programmes, carbon capture technologies, and renewable energies as a way to reduce carbon emissions and mitigate climate change. Hydrogen is a clean alternative to fossil fuels in automotive applications. In this context, the objective of this project is to find the best design of a hydrogen refuelling station in terms of the number of banks and their size, having as a final aim the most cost-efficient design. This study suggests that, from an economic point of view, a state of charge for the vehicle of 100% is not adequate, since it requires very large high-pressure banks at the station, which increases significantly its setup costs. The study finds that high-pressure banks have to be bigger in volume than the low-pressure banks to minimise the total cost of the station, including setup and operational costs along its timespan. Finally, the project shows that the optimal number of banks is 4 or a maximum of 5. As a side conclusion, these results have practical implications for firms, as they might reduce the time spent in the design process of a hydrogen refuelling station.

Introduction

Fossil fuels are the main culprits of anthropogenic carbon emissions increase and, therefore, climate change. Governments are promoting energy efficiency programmes, carbon capture, and renewable technologies to limit carbon emissions and mitigate climate change. In this context, hydrogen has been investigated for a long time as a clean alternative to hydrocarbon fuels in automotive applications. Hydrogen produces no emissions of CO_2 or air quality pollutants at the point of use. It has also a high specific energy storage capacity. These two characteristics make hydrogen an attractive alternative to fossil fuels for automotive industry. The potential transition from hydrocarbon-fuelled vehicles to hydrogen-powered vehicles requires a deep analysis of the technical and economic details of the hydrogen infrastructure, from the production of hydrogen to its delivery at the refuelling station. To make possible a transition to hydrogen vehicles, it is vital that consumers find hydrogen cars convenient to travel and easy and cheap to refuel. If there is no enough demand, automakers will not produce this type of cars and, logically, station-fuel providers will not invest in this technology.

To make the adoption of hydrogen vehicles easier, one of the most important challenges to overcome is a reduction in the cost of hydrogen [1,2]. The cost of hydrogen depends on the cost of the production, transportation and delivery. In the hydrogen vehicle market, refuelling stations are the major contributor to the total cost to customers, representing approximately half of the price [3]. The refuelling station costs are determined by the cost of the refuelling equipment and its running costs. Given the relevance of this issue, there is a need

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https://doi.org/10.1016/j.ijhydene.2018.11.001
0360-3199/

of investigating various hydrogen refuelling technologies, different components for a refuelling station and possible configurations to design a cost and energy efficient station, since an efficient hydrogen refuelling process is critical to favour the transition to clean and sustainable hydrogen vehicles.

This paper aims to find the optimal design of hydrogen refuelling station from a techno-economic point of view. In particular, the analysis pursues the most cost-effective design of the station in terms of the number and size of banks and energy consumed, by developing a practical MATLAB model. This model simulates the performance of a hydrogen refuelling station, following the protocol SAE J2061. This protocol was released by the Society of Automotive Engineers (SAE) and it contains technical information and standards describing the refuelling process for different vehicles' tanks in 2010. The main aim of the protocol is to achieve a refuelling process that satisfies the customers' needs without compromising safety [4]. To facilitate a potential transition to hydrogen vehicles, the refuelling process must be acceptable consumable, achieving all the desired customer attributes. Two important goals are: i) achieving a fast refuelling of approximate 3–5 min and ii) achieving a high state of charge (SOC) in the range of 90%–100% [5].

There are previous studies that have developed a computational model for a refuelling station, similarly to the one presented in this study, and studied on the energy and cost optimisation of hydrogen refuelling stations.

Rothuizen et al. [6] developed a thermodynamic station model to compare the energy consumption of the compressor and the refilling time of the banks for two different designs. They showed that the cascade system consumes less energy and reduces the refuelling time, being this statement a cornerstone for other studies. Using the same methodological approach, Rothuizen et al. [7] studied how different design parameters of a cascade system affected the energy consumption of the whole station. This study analyses the effect of adding more banks in the cascade system and the impact of changing the volume of the banks and their pressures, suggesting that the optimum number of banks is 3 or 4 for an energy-efficient design.

Omdahl [8] developed a similar model to the previous one, but it included an electrolyser for onsite production of hydrogen. The purpose of the study was to analyse the potential use of the heat wasted in an absorption refrigeration process to minimise the energy input of the station.

Talpacci et al. [9] also developed a thermodynamic model of the station to explore the most adequate cascade system to minimise the cooling energy. They showed that the low-pressure tank had to be smaller than the medium and high-pressure tanks to reduce the cooling energy.

Elgowainy et al. [10] uses a techno economic approach to minimise the total cost of a hydrogen station. They concluded that the hourly capacity of the compressor has to be twice the station average hourly demand and the cascade capacity 15% of the daily demand. Reddi et al. [11] maximise hydrogen utilisation at the lowest cost by optimising the compression and storage requirements. They showed that using a tube trailer to initially fill the vehicle can reduce the compressor and storage requirements thus reducing the refuelling cost.

Finally, Reddi et al. [3] carried out a relevant study on the cost of hydrogen. They conducted an analysis on which components of the station contributed the most to the refuelling cost. The results showed that the compressor, the refrigeration equipment and the storage vessels contribute the most to the station cost. To carry out the study, they used the Hydrogen Delivery Scenario Analysis Model (HDSAM), which was created by the H2A Analysis Group at the U.S. Department of Energy [12]. This model calculates the refuelling costs based on the refuelling design and delivery strategy. The cost information of each component is based on vendors, industry prices and engineering design calculations.

It is important to highlight that the study in this paper is inspired by Rothuizen et al. [7]. However, this study is different from Rothuizen et al. for two reasons. First, this project analyses the total costs of the station, including setup and energy costs (omitted by Rothuizen et al. [7]). Second, the optimisation of the volume of banks targets the most cost-efficient design. As it will be showed in this paper, the banks' volumes are one of the most relevant design consideration for the total cost of the station and the refuelling of the vehicle. To find the most cost-efficient combination in the size and number of banks, this study develops a thermodynamic model simulating the station operation. In the thermodynamic model, the heat losses from the banks to the surroundings are neglected and the hydrogen gas is considered a real gas.

The rest of the article is organized as follows: Modelling and methodology has a description of the model and the technical requirements that represent the physical constraints of the MATLAB model. Analysis and discussion of the results presents and discusses the results. Finally, Conclusion concludes.

Modelling and methodology

This following section explains the model of the station, including the relevant theoretical background and thermodynamic formulation.

Hydrogen refuelling system description

Hydrogen refuelling stations configuration can be divided in two parts: a dispenser system and a storage system. The aim of the dispenser system is to refuel the vehicle and its main components are the following. A high-pressure storage system that delivers fuel to the vehicle, a refrigeration system that precools the gas delivered and a dispenser that regulates the flow of gas into the vehicle [11]. The high-pressure storage consists of one or more banks and each of these have different pressures. The refuelling of the vehicle occurs from the lowest-pressure bank to the highest-pressure bank. This set up is known as a cascade system [7].

The main components of the storage system are a low-pressure hydrogen storage unit and a compressor that refills the high-pressure banks once a vehicle has been fuelled. There are several types of compressors that can be used, being reciprocating compressors or diaphragm compressors the standard ones. The most used compressor in hydrogen refuelling stations is a reciprocating compressor, which uses a piston to compress the hydrogen gas [7].

Modelling

The aim of the model is to predict the behaviour of the hydrogen gas across the station during the refuelling process. The necessary station components to comply with the SAE J206 are modelled using the first thermodynamic principles of mass and energy conservation.

Governing equation for the filling processes

The system for a simple hydrogen refuelling station can be described as the flow of gas going from the bank to the tank in the vehicle. Due to mass conservation principle, the mass leaving the bank at the station is the same as the mass received by the tank. The thermodynamics of both vessels (i.e. bank and vehicle tank) are determined applying the energy balance equation. Since the vessels have constant volume and no shaft work is performed, the equation for an open system is simplified to:

$$\frac{d(m_{gas}\,u_{gas})}{dt} = \dot{m}\,h_o + \dot{Q} \tag{2.1}$$

In Eq. (2.1), m_{gas} is the mass of gas inside the vessel, u_{gas} is the specific internal energy of the gas, h_o is the specific stagnation enthalpy, leaving or entering the system, $\dot{m}$ is the mass flow rate and $\dot{Q}$ is the rate of heat entering or leaving the system.

The hydrogen is delivered to the vehicle tank through a small delivery tube that protrudes into the cylinder. The gas flow occurs due to the pressure difference between the gas being delivered and the gas in the cylinder. The delivery tube can be modelled as an isentropic nozzle, assuming that there is no heat transfer and no work is done across it. Fig. 1 shows a sketch of the vehicle cylinder.

The mass flow rate of the gas at the inlet of the vehicle tank can be calculated using the isentropic mass flow rate equation:

$$\dot{m}_{ideal} = \rho_{static} V_{out} A_{out} \tag{2.2}$$

In Eq. (2.2), ρ_{static} is the static density at exit of the delivery tube, V_{out} is the velocity of the gas at that point and A_{out} is the cross-sectional area of the delivery tube. However, the isentropic assumption is not valid as there are irrecoverable losses due to the friction between the fluid and the delivery pipe [13]. Therefore, the actual mass flow can be obtained multiplying the ideal mass flow rate by a discharge coefficient.

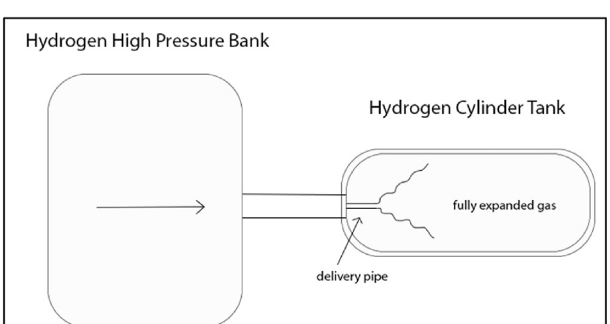

Fig. 1 – A schematic diagram of the vehicle tank during the filling process.

$$\dot{m} = C_D \dot{m}_{ideal} = C_D\,\rho_{static}\,V_{out}\,A_{out} \tag{2.3}$$

In Eq. (2.3), C_D is the discharge coefficient. This coefficient is primarily dependant on the Reynolds number and it can be expressed using Eq. (2.4) [14]. The most common definition of the Reynolds number is shown in Eq. (2.5).

$$C_D = I + \frac{J}{Re^n} \tag{2.4}$$

$$Re = \frac{\rho_{static} d V_{out}}{\mu_{out}} \tag{2.5}$$

In Eq. (2.4), I, J and the subscript n are constants and Re is the Reynolds number. These constants are found experimentally, and they are dependent on the type of nozzle and the conditions of the flow [15]. As a result, the discharge coefficient is affected by the viscosity of the fluid and the geometry of the nozzle. In Eq. (2.5), ρ_{static} is the static density at exit of the delivery tube, d is the diameter of the delivery tube, V_{out} is the velocity of the gas at the exit, and μ_{out} is the dynamic viscosity of the gas at the exit of the delivery tube.

The velocity of the gas at the exit of the delivery tube is calculated using the steady flow energy equation for an isentropic nozzle. It can be rearranged to give the velocity in the following form:

$$V_{out} = \sqrt{2(h_{o,in} - h_{out})} \tag{2.6}$$

In Eq. (2.6), $h_{o,in}$ is the upstream specific stagnation enthalpy which is calculated from the stagnation pressure and the stagnation temperature, h_{out} is the specific static enthalpy at the exit of the pipe obtained using the static entropy and the static pressure. The static entropy is obtained knowing that the static entropy is the same as the stagnation enthalpy and, therefore, it is equal to the stagnation entropy upstream. The static pressure is obtained by assuming that the gas is fully expanded at the exit of the delivery tube and, therefore, the static pressure at the exit of the tube is equal to the pressure of the gas inside the cylinder.

Modelling a compressor

Another critical component of a refuelling station is the compressor since moving the hydrogen from a low-pressure bank to a high-pressure bank requires mechanical work. The compression process can be assumed to be adiabatic, since the heat losses are usually 5% or less [16]. Therefore, the steady-state equation can be applied and simplified to this form:

$$\dot{W} = (h_{o,out} - h_{o,in})\dot{m} \tag{2.7}$$

In Eq. (2.7), $\dot{W}$ is the shaft work required for the compression of the hydrogen, $\dot{m}$ is the mass flow rate through the compressor and $h_{o,out}$ and $h_{o,in}$ are the specific stagnation enthalpy going out and in of the compressor, respectively.

The capacity of the compressor is given by the mass flow rate that is dependent on its design characteristics and it is given by:

$$\dot{m} = NV_{swept}\rho_{in}\eta_{V}n \tag{2.8}$$

In Eq. (2.8), N is the number of cylinders of the compressor, V_{swept} is the swept volume of the cylinder, n is the speed of the compressor measured in piston strokes per second, η_V is the volumetric efficiency and ρ_{in} is the density of the gas going inside the compressor.

The most commonly used compressor at hydrogen facilities is the reciprocating compressor [16]. This type of compressor uses the isentropic efficiency. Therefore, the total enthalpy going out of the compressor can be calculated using the isentropic efficiency:

$$h_{o,out} - h_{o,in} = \frac{h_{o,out,is} - h_{o,in}}{\eta_{is}} \tag{2.9}$$

In Eq. (2.9), $h_{o,in}$ is the enthalpy of the gas going inside the compressor, $h_{o,out,is}$ is the enthalpy corresponding to an isentropic compression. This is obtained from the pressure out of the compressor and the entropy entering the compressor.

The isentropic efficiency η_{is} is usually determined by experimental values. However, assuming is a reciprocating compressor, an estimate can be found using a formula where the value of the efficiency depends on the pressure ratio:

$$\eta_{is} = 0.1091\left(\ln\left(\frac{P_{out}}{P_{in}}\right)\right)^3 - 0.5247\left(\ln\left(\frac{P_{out}}{P_{in}}\right)\right)^2 + 0.8577\ln\left(\frac{P_{out}}{P_{in}}\right) + 0.3727 \tag{2.10}$$

In Eq. (2.10), P_{in} is the pressure going inside the compressor, i.e. the suction pressure, and P_{out} is the pressure going out, i.e. the discharge pressure. This equation is only valid for ratios between 1.1 and 5 [17].

Modelling a refrigeration system

The negative Joule-Thompson coefficient of hydrogen is responsible for an increase in gas temperature when it expands. An increase over 85 °C would cause structural failure in the vehicle tank. Therefore, one of the main safety regulations, ordered by the SAE J2061, is to precool the gas temperature down to −40 °C [5]. Typically, a refrigeration system is mainly composed of a heat exchanger and a compressor, which can be modelled separate.

Through the heat exchanger there is no work done and it can be assumed there are no pressure losses across it. Therefore, the steady-state energy equation can be applied and simplified to:

$$\dot{Q} = \left(h_{o,out} - h_{o,in}\right)\dot{m} \tag{2.11}$$

In Eq. (2.11), $\dot{Q}$ is the heat removal rate from the gas, $\dot{m}$is the mass flow rate through it, $h_{o,out}$ and $h_{o,in}$ are the specific stagnation enthalpy going out and in of the heat exchanger, respectively.

In practise, heat exchangers do not have an ideal performance. Hence, the cooled temperature is usually higher than expected. To calculate the real temperature going out of the heat exchanger, the effectiveness of the heat exchanger is needed. The equation for the effectiveness is the following:

$$\varepsilon = \frac{\text{Actual heat transfer}}{\text{Ideal heat transfer}} = \frac{h_{o,out,\ real} - h_{o,in}}{h_{o,out,\ ideal} - h_{o,in}} \tag{2.12}$$

In Eq. (2.12), ε is the effectiveness of the heat exchanger and $h_{o,out,\ ideal}$ is the specific stagnation enthalpy calculated from the ideal temperature. Once this value is found, $h_{o,out,\ real}$ can be obtained and, consequently, the actual temperature out of the heat exchanger.

To cool down the hydrogen, the compressor requires certain energy to drive the refrigerant across the heat exchanger. The energy consumed is dependent on the work needed to deliver the correspondent cooling temperature. They are related by the coefficient of performance as it can be seen in Eq. (2.13).

$$\dot{W} = \frac{\dot{Q}}{CoP} \tag{2.13}$$

In Eq. (2.13), $\dot{W}$ is the rate of work needed to apply to the refrigerator, $\dot{Q}$ is the heat removal rate and CoP is the coefficient of performance for refrigeration system. The refrigeration system is more efficient as the coefficient of performance increases. The CoP is dependent on the ambient temperature [18].

Modelling a piping system

The gas flows across the whole refuelling station, from the banks to the vehicle, through a piping system of interconnected pipes and valves. The piping system is modelled so that the pressure losses can be obtained. The pressure losses in the piping system can be broken down into: the major losses due to the friction and minor losses due to the valves and bends.

The total loss across the system can be modelled using the loss coefficients method assuming a constant diameter of the pipes. This method consists of simplifying each feature of the piping system to an equivalent pipe length achieving the same pressure loss [19].

$$P_{loss,\ total} = P_{loss,\ major} + P_{loss,\ minor} = \left(f\cdot\frac{L}{D} + \sum K_L\right)\frac{V^2}{2g} \tag{2.14}$$

The first term in Eq. (2.14) corresponds to the major loss due to the fiction along the pipe, where L is the length of the pipe, D is the diameter and f is the friction factor which can be calculated by using Colebrook equation [19]. However, Colebrook equation requires high computation time as it has to be use iteratively to find the friction factor. Consequently, the Haaland equation is used Eq. (2.15). This is an approximation formula that only differs by 2% respect to the Colebrook value [19]. In Eq. (2.15), the term $\varepsilon/_D$ represents the relative roughness of a pipe.

$$\frac{1}{\sqrt{f}} = -1.8\log\left(\left(\frac{\varepsilon/_D}{3.7}\right)^{1.11} + \frac{6.9}{Re}\right) \tag{2.15}$$

The second term in Eq. (2.14) corresponds to the sum of all the minor losses due to the valves and pipe bends, where K_L represents the loss coefficient of each feature of the piping system.

HDSAM cost model

The HDSAM model is used as a tool to calculate the total cost of the refuelling station. HDSAM model provides cost information for each component of the station for 2013 [12]. The cost data can be update to any year using the Chemical Engineering Plant Cost Index as it is shown in Appendix B: Cost Calculations. The HDSAM model also provides the formulas to calculate total energy costs along the lifetime of the station.

Model implementation

A simplified model of a hydrogen refuelling station with the necessary components to satisfy the SAE J2601 fuelling standard protocols is considered for this study. The model consists of two main systems: a storage system for refuelling the vehicle and the compressor system for refilling the banks at the station. Fig. 2 shows a graphical representation of the station model.

The set of equations presented on the previous sections constitute the model. The station model is divided in two parts, the refuelling system and the storage system composed of three banks with different working pressures. The initial properties for hydrogen gas inside the vehicle tank and the store system are known. The hydrogen refuelling station is considered to be model for vehicles with no communication. Therefore, the initial pressure of the vehicle and the ambient temperature are used to set the Average Pressure Ramp Rate (APRR) at the beginning of the process. The APRR and the target final pressure of the vehicle are specified by a series of "look-up tables" called TIR J2601 Look Up Tables which ensure the highest refuelling rate without violating safety [20].

Firstly, the reduction valve opens and controls the mass flow rate depending on the pressure inside the vehicle tank. At the beginning of the refuelling process, the station model opens the valve for the low-pressure bank in the cascade system and lets the gas flow to the vehicle. When the pressure across the reduction valve is too low to keep up with the APRR, the model switches to medium-pressure bank which has a higher pressure and the refuelling continues. Once again, when the pressure inside the bank is too low, the model changes to the high-pressure bank, until the vehicle tank satisfies one of the three conditions:

- The state of charge reaches 100%.
- The gas pressure inside the vehicle tank reaches a maximum filling pressure.
- The temperature inside the vehicle tank reaches the limit temperature of 85 °C.

Secondly, after the refuelling of the vehicle, the model is set up to replenish the banks at the station. The compressor delivers hydrogen gas from the low-pressure bank storage unit to the cascade system. The compressor fills the low-pressure bank first until it the gas pressure inside reaches the initial setup pressure, then the compressor changes to medium-pressure bank and high-pressure bank.

Finally, after both processes are finished, the model returns a cost analysis of the station. The model calculates the setup costs given the parameters of the station and the operating costs driven by the energy consumed.

Software used for the model

The model was developed and implemented in MATLAB and consists of a network of one-dimensional components interconnected. Each component at the station is written as an individual function. Each individual function receives the primary properties of the state of the gas (such as temperature and pressure) and it uses algebraic equations to evaluate the property state at the exit of the component. An explicit Euler integration has been implemented to solve the mass and energy balance of the gas in the tank of the vehicle and in the banks. Additionally, to account for the real gas effects, the property model REFPROP from the US National Institute of Standards and Technology (NIST) is used [21]. This model can determine any gas property from two independent properties.

Model assumptions

Technical assumptions

1. **Heat transfer between the vessels walls and the gas is neglected.** In practise, during the refilling, the gas is compressed and its temperature increases. The temperature difference between the gas and the vessel walls results in heat transfer. This phenomenon varies the actual gas temperature in the tank in a few degrees difference.

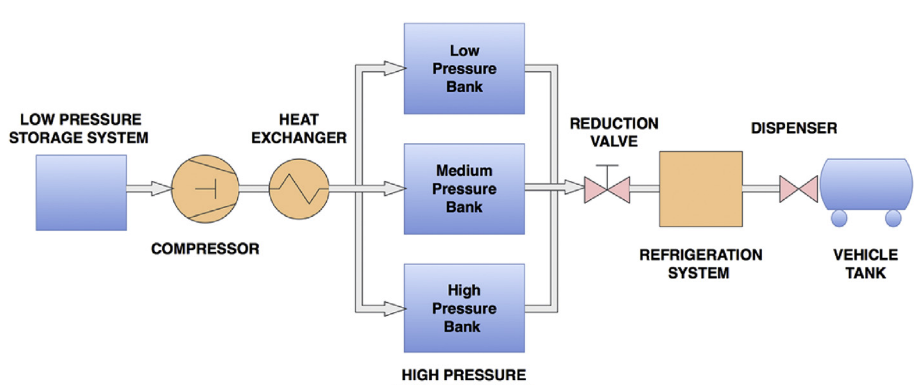

Fig. 2 – Sketch of the hydrogen refuelling station modelled in this study.

Knowing the exact gas temperature is not essential, given the aim of this study. However, it is necessary that the fuelling is achieved under the limit temperature, therefore, to ensure this, the gas is always cooled before delivering it.

2. **Pressure losses between the vehicle and the station are neglected.** These pressure losses are dependent on the type of tank being refuelled. To reduce the complexity of the model, it is assumed that the tank being refuelled always has the same the dimensions and properties. Therefore, pressure losses will be the same for all the scenarios analysed.
3. **Compressor and refrigerator unit can fulfil the demand.** The compressor has a constant throughput and it can refill the banks in any state. Its maximum flow rate is considered to be 30 kg/h, which corresponds to the peak mass flow capacity obtained when the pressure ratio is close to one. The refrigerator system can always achieve above the cooling demand.
4. **Only one car is being refilled at the time.** This assumption implies that the station has enough time to refill the banks before another car arrives for a refuelling. This assumption has an impact on the energy used to refill the banks. If the station has to refuel two or more cars consecutively, the compressor has to work for longer to compensate the lack of hydrogen inside the banks or the station needs a larger capacity compressor.

Economic assumptions

1. The total cost of the station is the sum of the cost of the investment and the discounted energy costs along the operational life of the station. In this study, the investment cost corresponds to the aggregate costs of the components of the station and the energy costs corresponds to the cost of running the station. Both costs are an estimate, so it might differ from other studies. Labour cost, the environmental cost, taxes, the property rent, and other different costs are not considered.
2. The price of energy is assumed to be constant along the timespan of the station. In practise, the price of energy can change over the years.
3. The energy costs are determined by the price of energy (electricity in this study) and the energy consumed by the station. The total energy consumed is the sum of the energy used to run the compressor to refill the banks plus the energy used to run the refrigerator system that cools down the hydrogen before being delivered.

Parameters specifications

The model receives technical specifications of the vehicle tank and the station as inputs (i.e. physical dimensions, initial temperatures and pressures), all these can be found in Appendix A: Model Parameters Specifications. The most important parameters are given here: i) The vehicle tank has a volume of 0.1224 m^3, corresponding to a hydrogen load of 5 kg ii) The initial pressure of the tank is 5 MPa iii) The ambient temperature is 20 °C and the APRR for these conditions is 21.8 MPa/min.

The cost of the high-pressure storage system was calculated using the data information in the HDSAM model. The estimated cost obtained for the storage capacity is £ 1150 per kilogram of hydrogen stored. The price of the dispenser, the compressor, the refrigerator and the storage system are calculated using HDSAM data.

The lifetime of the station is approximately 10 years [22]. The station refuels 50 cars per day per dispenser, which is an approximation for a Chevron gasoline refuelling station [11]. The estimated cost for electrical energy is £ 0.148 per kWh, which was obtained from Eurostat [23].

Validation of the model

This model has been validated using the results of Rothuizen et al. [7]. To validate the model, the station design previously showed in Fig. 2 is modified to be the same as the one presented by Rothuizen et al. [7]. Fig. 3 shows the energy

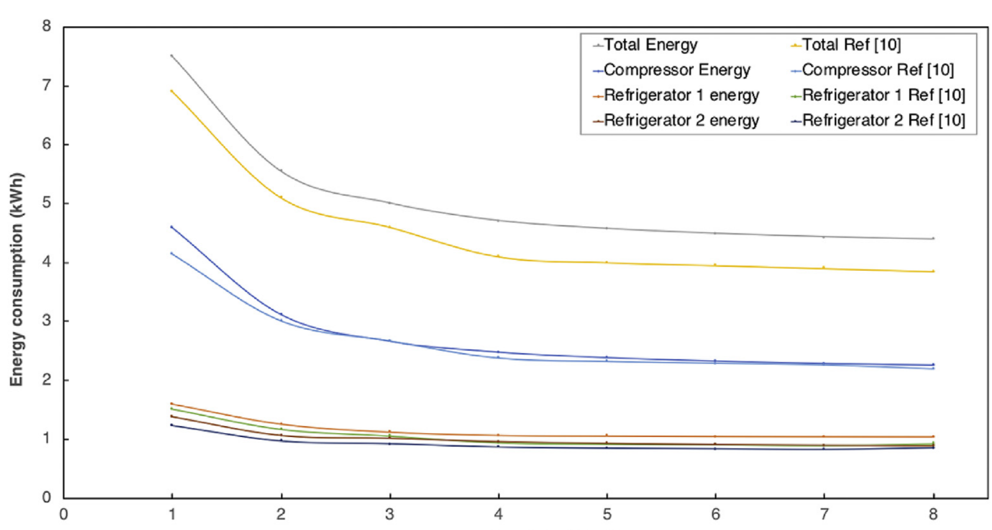

Fig. 3 – Comparative graph of the station components energy consumption between the MATLAB model and the model by Rothuizen et al. [7].

consumption for each of the components of the station for different number of banks for Rothuizen et al. [7] and this MATLAB model.

The trend of the energy consumed when adding more banks follows the one by Rothuizen et al. [7]. For the objective of this study, very precise values are not extremely important, as the study focuses on total cost over the timespan of the station. For this reason, the MATLAB model is close enough to the reference paper, providing confidence in the simulation results of this project.

Analysis and discussion of the results

In the following section, the thermodynamics of the system are analysed. An optimisation of the volume of the banks of the cascade system is analysed for the SOC, the setup cost and the energy cost, additionally, an optimal configuration for the cascade system is obtained. The total volume of the cascade storage is in the range of 0.25 m^3–11 m^3 for all simulations, ensuring always a complete refuelling of the vehicle. The refuelling processes carried out in this section are simulated in accordance with SAE TIR J2601.

Thermodynamic study

In order to explain the thermodynamic properties of the system, the complete refuelling cycle of a three banks cascade station is used as a reference. The low-pressure bank (40 MPa), the medium-pressure bank (65 MPa) and the high-pressure bank (90 MPa) are 1.5 m^3, 1.5 m^3 and 2 m^3, respectively, to ensure a fuelling of a SOC of 100%. The ambient temperature is 20 °C. Fig. 4 shows the evolution of the main thermodynamics properties on the tank vehicle and on the cascade system.

As seen in Fig. 4(a) the pressure inside the tank vehicle increases according to the APRR, since the pressure losses in the vehicle storage system are neglected. The fuelling continues until it reaches a SOC of 100% after 235.48 s and always below the safety limit pressure of 87.5 MPa. This is approximately 4 min and it is considered a fast refuelling time. The pressure graph also shows two changes in pressure, corresponding to the time where the cascade system switches bank.

Fig. 4(b) shows the temperature evolution and shows that the gas temperature inside the tank of the vehicle ramps up very quickly, due to the negative Joule Thompson coefficient of hydrogen. To fulfil the protocol safety requirements, the refrigerator is positioned after the reduction valve to cool down the hydrogen to −40 °C, thus not exceeding the gas limit temperature (85 °C) during the refuelling.

Fig. 4(c) shows the mass flow rate and the cooling demand. The cooling demand is a function of the mass flow and the enthalpy, as seen in Eq. (2.11). Therefore, its slope is similar to the one of the mass flow rate. A rapid rise in cooling takes place when the station switches to a higher-pressure bank.

Finally, Fig. 4(d) and (e) shows the evolution of pressure and temperature of the banks during the complete refuelling cycle, respectively. After the refuelling of the vehicle, the banks are refill to their original working pressures and correspond to a linear refill determined by the mass flow rate of the compressor. The pressure drop in the banks during the refuelling, leads to an expansion of the gas and consequently a rapid decrease in temperature. The temperature remains constant because it is assumed that there is no heat transfer between the walls of the banks. The temperature rapidly increases again when the banks are refilled.

Results: the effect of the bank volume on the state of charge

The model was initially tested for the refuelling of a car with the gas being delivered from a station with one bank at a fixed initial pressure. The initial pressure of the bank is 90 MPa since it is the recommended working pressure for high-pressure banks of type III and type IV in hydrogen storage systems [16]. The state of charge (SOC) of a vehicle tank depends on the volume of the bank at the station as it is shown in Fig. 5.

Fig. 5 shows that the minimum bank volume to achieve a 100% SOC is 7.25 m^3. It also shows that a bigger bank (in volume) leads to a higher SOC. Once the SOC reaches around 95%, a higher SOC requires a quite large increase in the volume of the bank. The reason for this is that as the refuelling takes place, the gas pressure inside the tank of the vehicle increases. This increase makes the refuelling more difficult, implying that more mass of hydrogen is needed to rise the gas pressure. At the same pressure, a smaller bank contains less mass than a bigger bank. So, in conclusion, a much bigger bank is needed, as a higher SOC is required.

According to the HDSAM model seen in HDSAM cost model, the volume of the banks affects the setup costs since the price of the storage system will vary accordingly to its total capacity. The setup cost of the storage system is a linear function of the total volume. Therefore, the smaller the total volume is, the lower the setup cost and thus, a lower total cost of the station.

The main take away from these observations is that, from a cost-efficient point of view, for a station with one bank, once the tank of the vehicle has achieved 99% of SOC, achieving 100% requires nearly doubling the set-up costs. However, the optimal SOC would be a trade-off between the station costs and the customer needs, in other words, how much would the driver would be willing to pay to increase the range of his vehicle. This study assumes that the station will recharge 50 Toyota Mirai per day over a period of 10 years (lifespan of the station) each of them with a driving range of 650 km.

Fig. 6 shows how different values of the SOC affect the driving range per refilling and the setup cost that the owner of the station must charge per km travelled. Given that the owner of the station has to charge the setup costs to the customers to recover his investment, the cost per kilometre is equal to the setup cost divided by the total driving range (assuming no profit). An increase in 1% of the SOC increases linearly the range of the vehicle by 6.5 km, while it increases exponentially the setup cost per kilometre travelled.

Fig. 6 illustrates that the setup cost per kilometre travelled is almost constant until it reaches 95%. This would be the most cost-efficient SOC, however, the impact on the car driving range would be high. The choice of the “optimal” SOC will depend on the customer willingness to pay more to expand the range of his vehicle. Finding the right balance

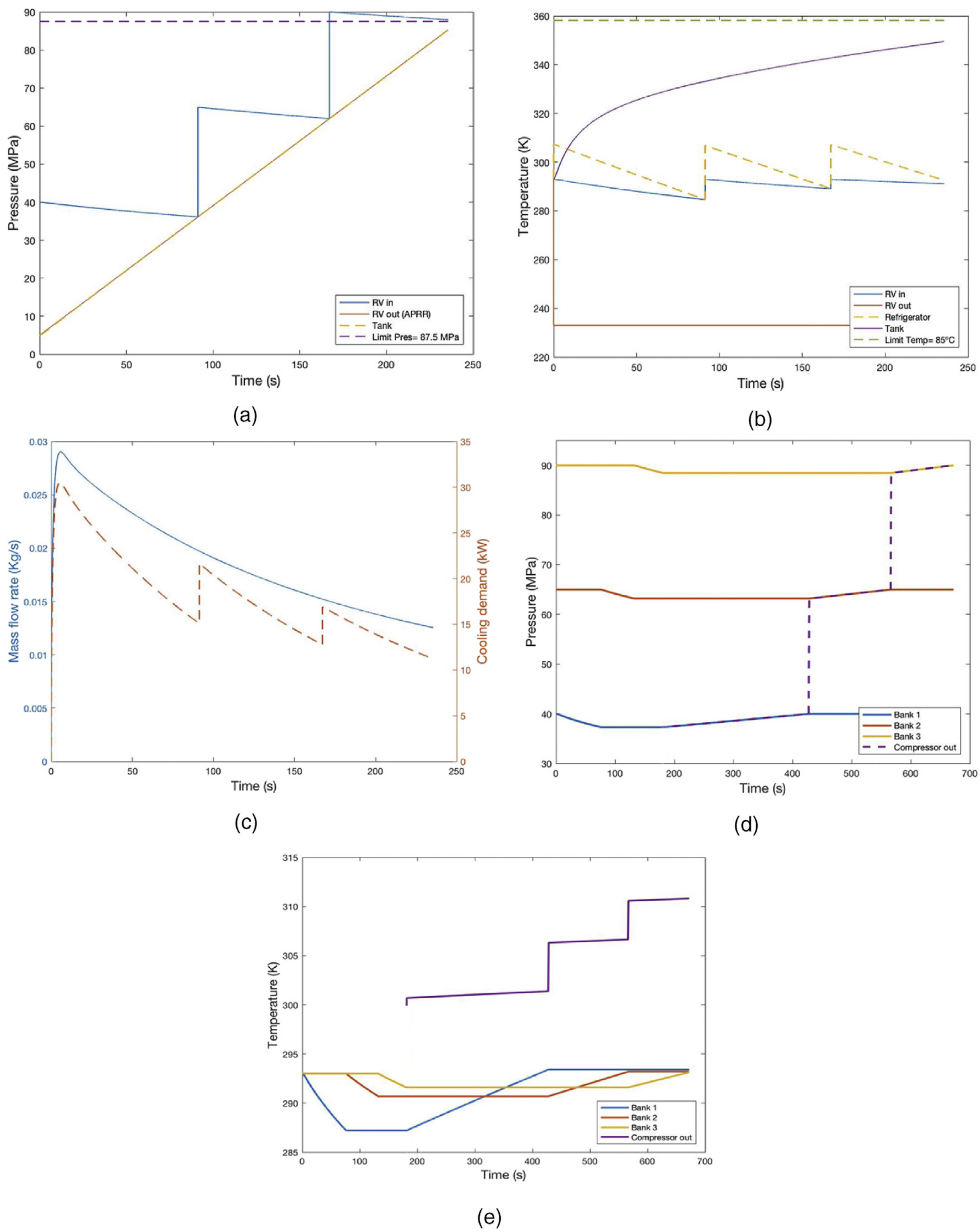

Fig. 4 – Evolution of thermodynamic properties in the components showed in Fig. 2. (a) Pressure in the system when refuelling the vehicle (RV is the Reduction Valve). (b) Temperature in the system when refuelling the vehicle. (c) Mass flow and cooling demand when refuelling the vehicle. (d) Pressure inside the banks in the cascade system and compressor (Bank 1 = Low-pressure, Bank 2 = Medium-pressure, Bank 3 = High-pressure). (e) Temperature inside the banks in the cascade system and compressor (Bank 1 = Low-pressure, Bank 2 = Medium-pressure, Bank 3 = High-pressure).

between both variables based on consumers' preferences is out of the scope of this study.

Given that the scope of this study is to conduct a techno-economic analysis and the sharpest increase in the setup cost takes place when the SOC shifts from 99% to 100%, this study considers a SOC of 99% as an adequate value from an economic point of view. This implies that the effective range of the Toyota Mirai is 643.5 km rather than 650 km and that the required volume for one bank at the station at 90 MPa is 4.60 m^3 rather than 7.25 m^3. In any case, the main qualitative

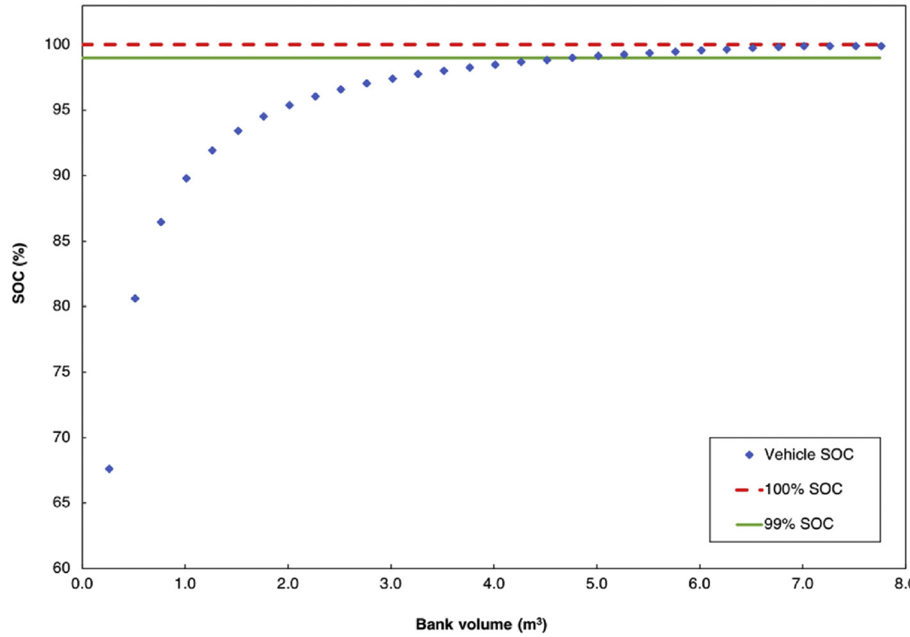

Fig. 5 – The state of charge of a vehicle depending on the volume of the bank in the station.

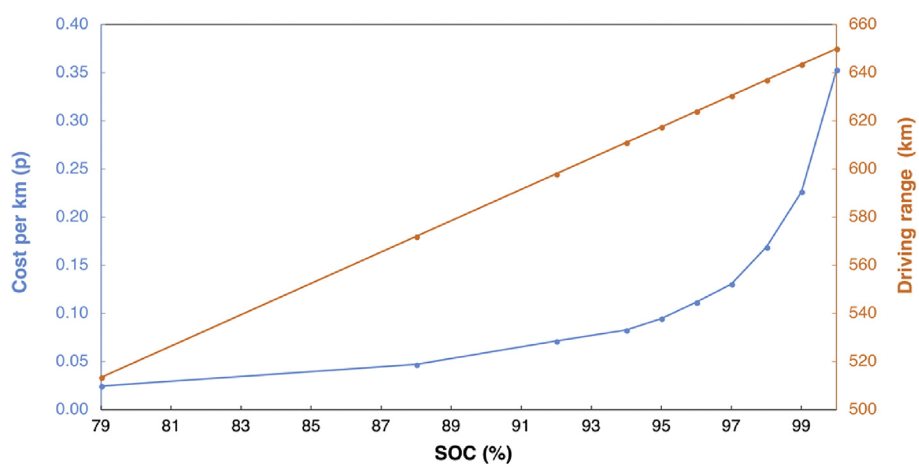

Fig. 6 – The effect of the SOC of the vehicle on the driving range (orange) and on the cost per kilometre travelled (blue). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

results of this study hold for any reasonable SOC (between 95% and 99%).

Results: effect of the bank volume on setup and energy costs

The station model has now two banks rather than one: a low-pressure bank (Bank 1) and a high-pressure bank (Bank 2), with their corresponding volumes V_1 and V_2. The pressures of the two banks are 40 MPa and 90 MPa, respectively.

The setup cost of the station depends on the total capacity of the storage system, and thus, the volume of the banks. To minimise the aggregate volume, different combinations of volumes of Bank 1 and Bank 2 have been modelled. In the previous section, the results showed that, when the station has only one bank, achieving a SOC above 95% required an exponential increase in the setup cost. This evolution of the setup cost resulted in a higher driving range, but the cost per kilometre travelled increased also exponentially. To verify whether this statement is satisfied for multiple banks, a similar analysis is conducted for a station with two banks with different combination of sizes.

Fig. 7 shows the results of the analysis. It can be observed that even with two banks in the station, the higher the SOC the exponentially higher setup cost. The setup up cost increase by nearly a factor of two when the SOC shifts from 99% to 100%. This analysis confirms that for more than one bank 99% is still an adequate value from an economic point of view. As in the case of one bank, the choice of this technical parameter is driven by an economic motivation. To sum up, this study assumes that a SOC of 99% is a complete refuelling.

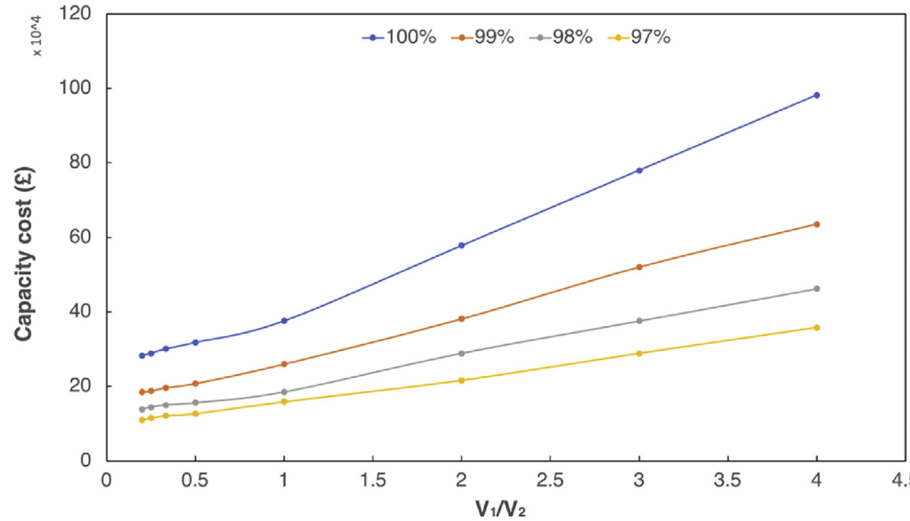

Fig. 7 – Storage setup costs for different SOC and different combinations of volumes of Bank 1 (40 MPa) and Bank 2 (90 MPa).

Table 1 shows the total volume for a complete refuelling for each combination and the change in volume relative to the previous case (for example, case 3 respect to case 2).

Table 1 indicates that the aggregate minimum volume increases as the low-pressure bank volume (V_1) gets bigger. The reason for this is the mass of hydrogen drawn to the vehicle has to be the same. When the two banks have the same volume, the bank at a higher pressure contains more mass than the bank at a lower pressure. If Bank 2 is smaller than Bank 1, the amount of mass stored in the banks decreases considerably. Therefore, Bank 1 will have to highly increase in volume until the mass of gas inside is enough to complete the refuelling. In conclusion, the aggregate volume (V_1+V_2) required is less when you have a bigger Bank 2 since it can store more mass than Bank 1 given the same volume.

The minimum total volume converges to a value of around 3.20 m^3, for the given pressures of 90 MPa for the high-pressure bank and 40 MPa for the low-pressure bank. Theoretically, the most appropriate volume distribution for two banks to achieve the minimum set up cost is that the high-pressure bank is as big as possible compared to the low-pressure bank. However, this would result in a low-pressure bank volume too small making it unrealistic for practical applications. Therefore, the most practical combination is that the high-pressure bank is 4 times bigger than the low-pressure bank.

The different combinations of volumes of the banks also affect the total energy consumption of the station, i.e. the sum of the energy used to run the compressor plus the energy used to run the refrigerator. Table 2 shows the different combinations of banks, the total energy consumed, and the change in energy relative to the previous case. Table 2 points out that the total energy consumption decreases as the volume of Bank 1 increases. It can be seen that the change in energy relative to the previous case is very small in all the cases.

Total energy consumption can be separated into energy consumed by the compressor and energy consumed by the refrigerator. Fig. 8 shows the energy consumption of the compressor for each bank for every combination of volumes. Total energy consumption of the compressor increases as Bank 2 gets bigger (from Case 5 to Case 8). The reason is that the energy consumed by the compressor (measured in kWh) depends on the compressor power and its operating time. The compressor power increases when the pressure ratio between the inlet and the outlet increases. Therefore, the power needed is higher when a high-pressure bank is refilled. The operating time of the compressor depends on the amount of mass that the bank needs to be completely full. For this

Table 1 – Different combinations of volumes of Bank 1 and Bank 2, the total volume of both banks and the change in volume for each case.

	Different combinations of volumes	Total minimum volume (m^3)	Change in total minimum volume (%)
Case 1	$V_1 = 4V_2$	11.00	–
Case 2	$V_1 = 3V_2$	9.00	18.18
Case 3	$V_1 = 2V_2$	6.60	26.67
Case 4	$V_1 = V_2$	4.55	31.06
Case 5	$V_1 = V_2/2$	3.60	20.88
Case 6	$V_1 = V_2/3$	3.40	5.56
Case 7	$V_1 = V_2/4$	3.25	4.41
Case 8	$V_1 = V_2/5$	3.20	1.54

Table 2 – Different combinations of volumes of Bank 1 and Bank 2, total energy consumed and the change in energy for each case.

	Different combinations of volumes	Total energy consumption (kWh)	Change in energy consumption (%)
Case 1	$V_1 = 4V_2$	3.58	–
Case 2	$V_1 = 3V_2$	3.59	0.03
Case 3	$V_1 = 2V_2$	3.59	0.02
Case 4	$V_1 = V_2$	3.59	0.20
Case 5	$V_1 = V_2/2$	3.61	0.52
Case 6	$V_1 = V_2/3$	3.63	0.62
Case 7	$V_1 = V_2/4$	3.65	0.47
Case 8	$V_1 = V_2/5$	3.67	0.51

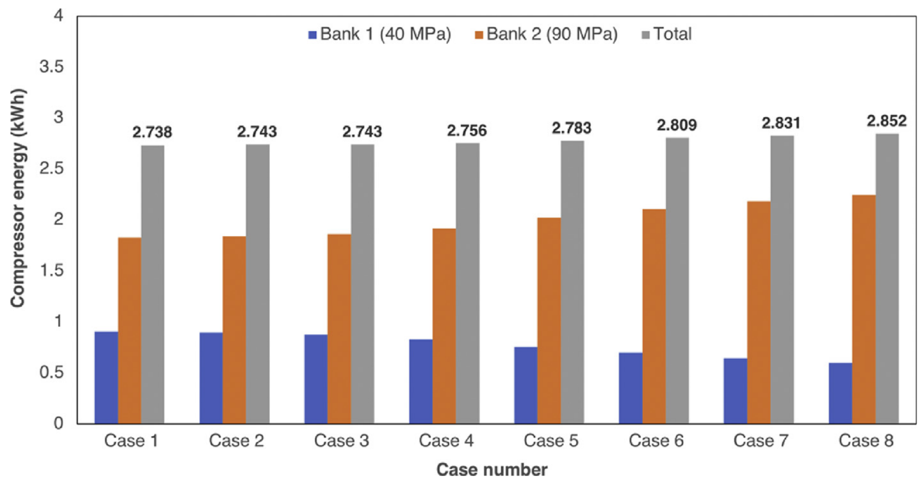

Fig. 8 – Energy consumed by the compressor to refill Bank 1 and Bank 2 for each combination of volumes.

reason, when Bank 2 is bigger, the compressor has to refill more amount of mass at a higher pressure, increasing the energy consumed.

The energy consumption of the refrigerator for each bank for every combination of volumes is shown in Fig. 9. The negative rate of growth of the total energy is the result of two variables. One variable is the positive increase in energy consumption due to an increase in the size of the high-pressure bank (Bank 2, from Case 1 to Case 8), which causes an increase in the pressure difference across the reduction valve and thus, the Joule-Thompson effect increases the temperature of hydrogen. The second variable is the negative decrease in energy consumption due to a decrease in the size of the low-pressure bank (Bank 1 from Case 1 to Case 8) and thus, the decrease of aggregated volume and amount of hydrogen. Fig. 10 shows the change in energy consumption for Bank 1 (decrease) and for Bank 2 (increase) for every case. The graph shows that the negative variable grows at a faster rate that the positive variable, resulting in a decrease of the overall energy consumption. The figure has the rate of growth in absolute terms to make easier the visual analysis.

Finally, and going back to Table 2, total energy consumption follows an opposite trend as the energy consumed by the compressor, decreasing as Bank 2 gets bigger. However, the energy consumed by the refrigerator is small, having no significant effect on the trend of total energy consumed by the station. From an energy consumption point of view, the station should have a low-pressure bank as big as possible. However, from a practical perspective, the appropriate volume distribution is to have the low-pressure bank 4 times bigger than the high-pressure bank.

It has been concluded that the volume distribution of the banks to minimise energy consumption and to minimise setup cost is different. This is a relevant conclusion. Given that the aim of this study is to design a cost-efficient station, to make a decision it is necessary to sum both costs. The setup cost is an investment cost that takes place initially, when the station is built-up. On the contrary, the energy consumed is a cost that runs along the life of the station. The setup cost is simply the aggregated volume of Bank 1 and Bank 2 multiplied by the price. The total cost of the energy is the aggregated energy used to refuel 50 cars per day over a period of 10 years,

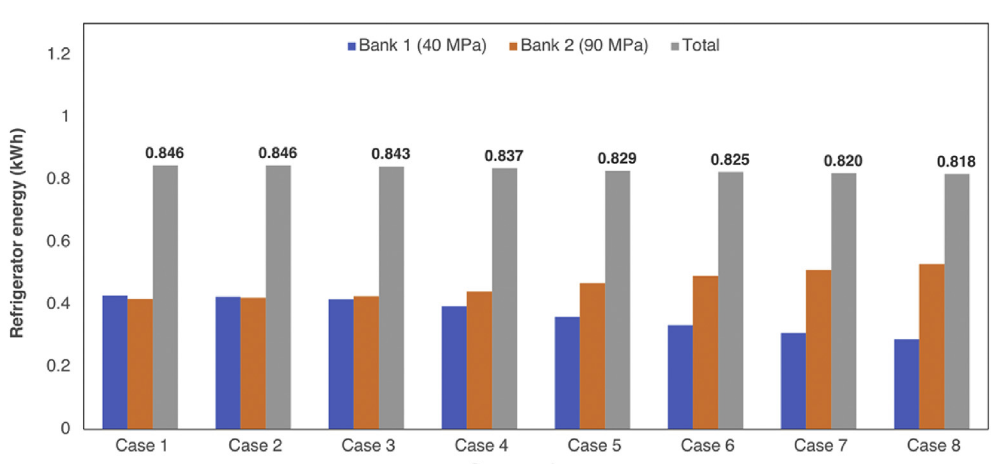

Fig. 9 – Energy consumed by the refrigeration unit to cool down the gas to −40 °C for each bank for each combination of volumes.

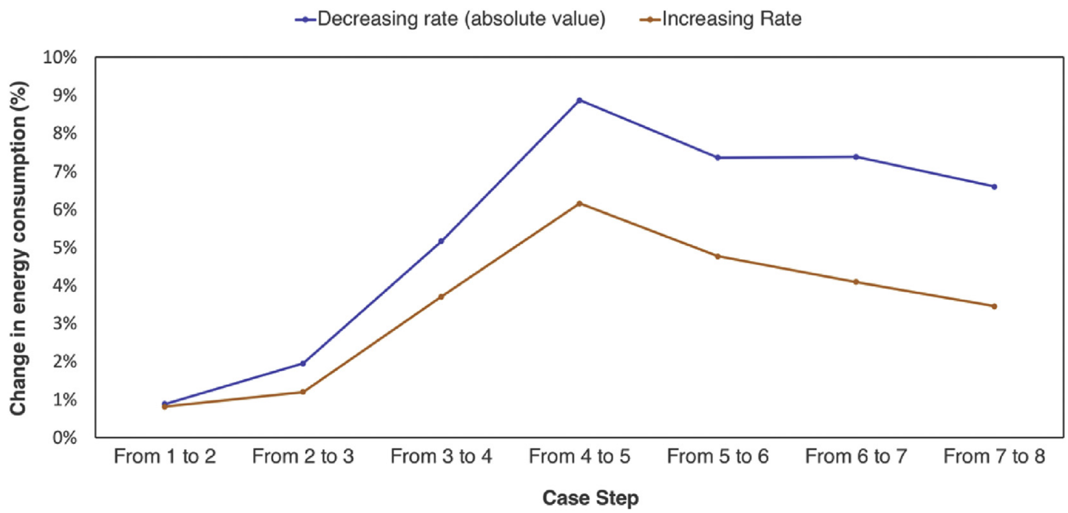

Fig. 10 – The change in energy consumption for Bank 1 (decrease rate) and for Bank 2 (increase rate) for each case.

which is the lifespan of the station, multiplied by the price of energy. As it is standard in the evaluation of investment projects, the total cost is the discount of the sum of all the costs along the lifespan of the project [24]. In this case, the cost of the station is the sum of the setup costs plus the discounted of the cost of the energy consumed along the timespan of the station. See Appendix C: Discounted Cost of the Energy Consumed of a detailed description and implementation of this variable.

Table 3 – Setup initial pressure for each bank for different number of banks.

Number of banks	Bank 1 (MPa)	Bank 2 (MPa)	Bank 3 (MPa)	Bank 4 (MPa)	Bank 5 (MPa)	Bank 6 (MPa)
1	90.00	–	–	–	–	–
2	40.00	90.00	–	–	–	–
3	40.00	65.00	90.00	–	–	–
4	40.00	56.67	73.33	90.00	–	–
5	40.00	52.50	65.00	77.50	90.00	–
6	40.00	50.00	60.00	70.00	80.00	90.00

Fig. 11 shows the total cost of the station over its lifetime for the different volumes combinations. The relevant variable that determines the total cost of the station is the setup cost and, therefore, the total storage volume. In conclusion, and again for a practical application, an optimal distribution for a station with two banks would be the one that has a high-pressure bank 4 times bigger than the low-pressure bank.

Results: Optimal configuration of a cascade system.

This section finds the optimal combination of banks (in number and size) for a station. The optimisation is done for a station model with multiple banks, from 1 to 6. The pressures of the banks are shown in Table 3. The pressures are linearly distributed between 40 MPa and 90 MPa with an equal pressure rise.

The addition of more banks multiplies exponentially the number of potential combinations of volumes. To select the appropriate combination to minimise the total cost, the results from the previous section are used as a guide. The first insight is that the cost of energy plays a minor role in determining the total cost of the station. For this reason, and to

Table 4 – Combination of volumes 3 and 4 for different number of banks.

Number of banks	Combination 1	Combination 2
1	V_1	V_1
2	$V_1 = V_2/2$	$V_1 = V_2/4$
3	$V_1 = V_2 = V_3/2$	$V_1 = V_2 = V_3/4$
4	$V_1 = V_2 = V_3 = V_4/2$	$V_1 = V_2 = V_3 = V_4/4$
5	$V_1 = V_2 = V_3 = V_4 = V_5/2$	$V_1 = V_2 = V_3 = V_4 = V_5/4$
6	$V_1 = V_2 = V_3 = V_4 = V_5 = V_6/2$	$V_1 = V_2 = V_3 = V_4 = V_5 = V_6/4$
Number of banks	**Combination 3**	**Combination 4**
1	V_1	V_1
2	$V_1 = V_2/2$	$V_1 = V_2$
3	$V_1 = V_2/2 = V_3/3$	$V_1 = V_2 = V_3$
4	$V_1 = V_2/2 = V_3/3 = V_4/4$	$V_1 = V_2 = V_3 = V_4$
5	$V_1 = V_2/2 = V_3/3 = V_4/4 = V_5/5$	$V_1 = V_2 = V_3 = V_4 = V_5$
6	$V_1 = V_2/2 = V_3/3 = V_4/4 = V_5/5 = V_6/6$	$V_1 = V_2 = V_3 = V_4 = V_5 = V_6$

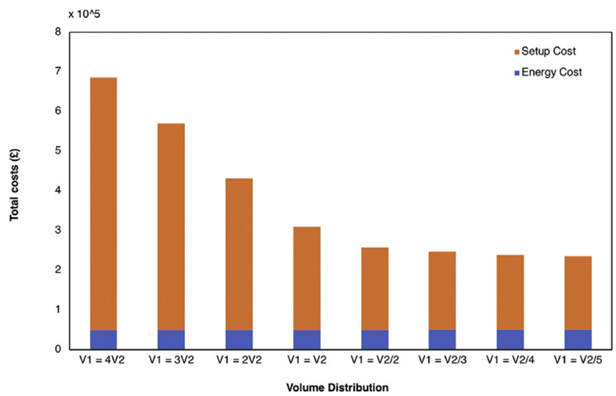

Fig. 11 – Total cost of the station over its lifetime for each combination of volumes.

minimise the total cost of the station, the objective of this section will be to minimise the total volume. The second insight is that the high-pressure bank has to be bigger than the low-pressure bank to achieve the cost objective.

Table 4 shows all the combinations analysed. In Combination 1 and Combination 2 the highest-pressure bank is two and four times bigger than the other banks, respectively. Combination 3 is a linear distribution of volumes, with the largest bank at the highest pressure. Finally, Combination 4 is the case where all volumes are equal. This combination is used as a reference. It has to be noticed that for two banks, Combination 1 and 3 are the same.

Fig. 12 shows the minimum aggregated volume of the banks to achieve a SOC of 99% for each combination. The combination that gives the minimum volume for any number of banks is

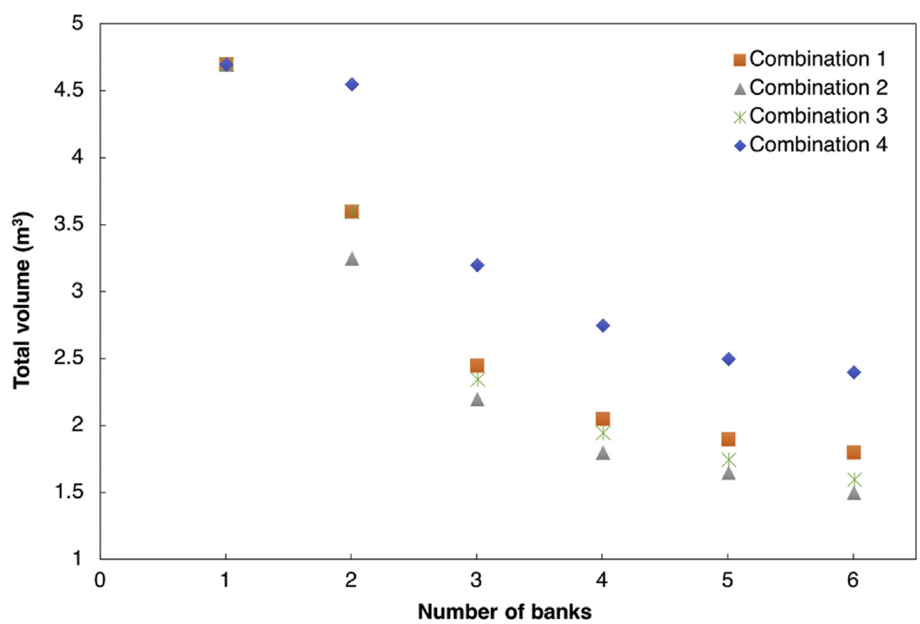

Fig. 12 – The minimum total volume for a complete refuelling for each volume combination for different number of banks.

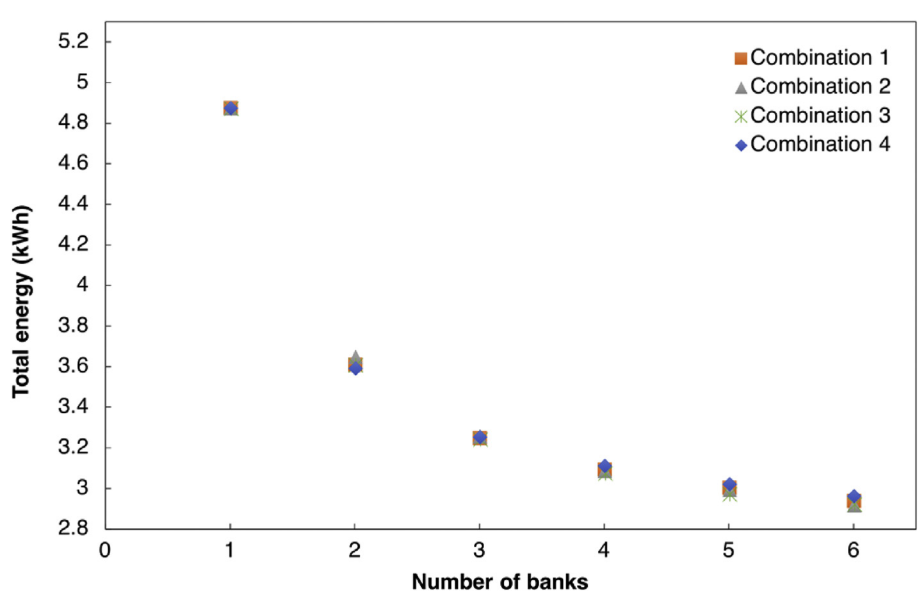

Fig. 13 – The total energy consumption for a complete refuelling for each volume combination for different number of banks.

Combination 2, where the highest-pressure bank is four times bigger than the rest of the banks. For Combination 2, as the number of banks in the station increases, the total volume decreases and converges to a value of 1.60 m^3. As the number of banks increases, the volume of each individual bank will get smaller. For this reason, to avoid banks that are too small and considering all the techno-economic assumptions made in this project, a practical solution to minimise the setup storage cost is to have a station with 4 or a maximum of 5 banks (5 banks could also be a cost-effective design, but the individual sizes of the banks could be too small and unrealistic for practical applications) arranged in this volume distribution.

For the sake of completeness, Fig. 13 shows the total energy consumption for each combination. The difference in energy between the combinations is very small. The combination that gives the minimum total energy consumption for all cases is Combination 3, which corresponds to the linear distribution of volumes. However, as it is seen in the previous section, the small difference in energy is not a decisive variable of the total cost of the station (see Fig. 11).

Conclusions

The objective of this project is to find the optimal design of a hydrogen refuelling station from an economic point of view. In particular, this study explores different design in terms of the number of banks and their size, having as a final objective the most cost-efficient design. The simulation model is inspired Rothuizen et al. [7], but with substantial modifications regarding the size and number of the banks. In particular, this study analyses 32 different banks configurations to answer the research question. The station model is developed and implemented in MATLAB.

This study has the three relevant insights. First, from an economical point of view, a state of charge of 100% is not adequate since it requires a very large bank increasing significantly the cost of the station and thus, the cost per kilometre travelled for the customer. This study considers a state of charge of 99% as a cost-effective alternative.

Second, the high-pressure bank (or banks) has to be bigger in volume than the low-pressure bank (or banks) to minimise the total and set up costs. This type of configuration is not effective in terms of the energy consumed, since there are alternative designs that consume less energy such as a linear distribution of volumes. However, this study shows that the economic cost of the energy used along the lifespan of the station is not very relevant compared to the setup costs. For the sake of simplification of the analysis, this study does consider other costs such as lands rents, labour costs, environmental permissions, etc. In addition, these costs are independent from design of the station, being identical in all the cases.

Third, there is an optimal configuration of the banks. In particular, the optimal number of banks is 4 or a maximum of 5, where the highest-pressure bank has to be 4 times bigger in volume than the rest with a total volume of 1.60 m^3 (1600 l). Adding more banks reduce marginally total cost of the station, but at the cost of higher complexity.

As a side conclusion, it can be highlighted that these results have practical implications. Commercials firm developing a project of a hydrogen refuelling station can use the results of this research as a starting point of the designing process.

Finally, this study assumes that the price of electricity in the UK is constant in time. A potential expansion of this study is to conduct a sensitivity analysis to explore to what extent these results are robust to variations in the price of electricity.

Acknowledgements

I would like to thank my supervisor Dr Edward S. Richardson for his guidance and support throughout the course of this project. I am also grateful for the suggestions from various colleagues of Southampton University. Finally, I am grateful to two anonymous referees and the editor for their recommendations and comments that have helped to improve considerably the paper. Nonetheless, I am responsible for all errors and omissions. Furthermore, the views expressed in this paper are those of the author and do not necessarily represent the views of her affiliated institution.

Appendix A. Model parameters specifications

Model parameters specifications

Tank technical parameters

Table A.1 – Model parameters for the 2016 Toyota Mirai. From Ref. [25].

Volume tank	0.1224 m^3
Storage capacity	≈5 kg
Nominal pressure	70 MPa
Maximum filling pressure	87.5 MPa
Driving range	≈650 km
Initial tank pressure	5 MPa

Station technical parameters

Table A.2 – Model parameters for the station [20].

Ambient Temperature	20 °C
Pre-cooling temperature	−40 °C
APRR	21.8 MPa/min

Valve parameters

Table A.3 – Loss coefficient for different features of the piping systems. From Ref. [19].

Ball valve	$K_L = 0.05$
Control valve	$K_L = 10$
90º Bends	$K_L = 0.3$

Appendix B. Cost calculations

This section calculates the estimated cost for the components of a refuelling station using the data information from the HDSAM model [12]. As explained in HDSAM cost model, the cost data information provides the prices of the components for 2013. To update the costs to 2016, the Chemical Engineering Plant Cost Index of 2017 needs to be used. Eq. (B1) shows how the updated price is obtained.

$$price_{2016} = price_{2013}\frac{index_{2016}}{index_{2013}} \tag{B1}$$

The HDSAM model provides the prices of the components in dollars. To obtain an estimate in pounds, the value used for the conversion is 1 Dollar to 0.72 Pounds. The following table shows the original values from the HDSAM and the estimates used for this project for each component.

Components	HDSAM 2013	MATLAB Model 2016
High-pressure storage	1800 \$/kg	1150 £/kg
Low-pressure storage	1200 \$/kg	770 £/kg
Heat exchanger	25,000 \$/unit	16,000 £/unit
Dispenser	100,000 \$/unit	67,000 £/unit
Compressor[a]	40,035 \$/kW	33,800 £/kW

[a] The compressor cost depends on its capacity (in kW) and it is governed by Eq. (B2).

$$\text{compressor}_{\text{cost}} = 40035\ (\text{capacity})^{0.6038} \tag{B2}$$

Appendix C. Discounted cost of the energy consumed

This study designs a hydrogen station from cost efficient perspective. Setup costs take place in the first moment, when the station is build up. However, energy costs take place in every refuelling and for a period of 10 years. The sum of discounted costs is the standard way to add costs that take place in different moments of time [24].

The cost of the station is, then, the sum of all discounted costs for a period of 10 years, according to the following formula.

$$\sum_{t=0}^{10} \frac{car_t * e * p_t}{(1+r)^t} + Setupcost \tag{C3}$$

where, t represents time, the variable car_t is the number of cars refuelled at time t (which is constant in this study), e is the energy consumed per refuelling, p_t is the price of energy at time t (which is constant in this study), and r is the discount rate. The discount rate used is 7.5%. This is the one used by IRENA to assess the cost of the renewable energy projects in developed countries [24]. The first part of the formula represents the energy cost in this study.

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