PROCEEDINGS OF ECOS 2023 - THE 36TH INTERNATIONAL CONFERENCE ON
EFFICIENCY, **C**OST, **O**PTIMIZATION, **S**IMULATION AND ENVIRONMENTAL IMPACT OF ENERGY SYSTEMS
25-30 JUNE, 2023, LAS PALMAS DE GRAN CANARIA, SPAIN

Development of a numerical optimization model for sizing hydrogen refuelling stations: application to a case study

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Abstract:

Interest in hydrogen as a transportation fuel is growing. Fuel cell electric vehicles fed by hydrogen are expected to play a key role in the decarbonization of the transportation sector. Its impact will depend upon the existence of reliable and cost-effective fuelling stations. Numerical simulation allows sizing hydrogen refuelling on-site stations in order to identify the most cost-effective solution for a specific utilization pattern. This study aims to define a numerical optimization model for a hydrogen refuelling station to supply both light and heavy vehicles. The objective function is to minimize the total storage volume, taking into account the number of vehicles to be refuelled. The pressure at each storage skid is considered a decision variable, as well as the hydrogen mass that is provided at each vehicle filling. The model considers the hydrogen properties and the physical constraints to size the station prior to its construction. Additionally, a cost analysis based on the capital expenditure concept was developed. The hydrogen refuelling station must be able to supply 300 kg/day of hydrogen. The station includes four main systems: the hydrogen production equipment, an electrolyzer, and a system that can store hydrogen to feed the compression cascade. The station should be able to fill 10 heavy vehicles at 350 bar (H35), considering 2 skid pressure levels and a supplied mass of 30 kg and 30 light vehicles at 700 bar (H70), considering 3 skid pressure levels, dispensing 4.2 kg of hydrogen each. At all vehicle fillings, a pressure differential of 50 bar between the high-pressure skid and the vehicle tank is mandatory so the refuelling can be validated. The results show that it is possible to refuel 10 heavy vehicles considering a total storage volume of 36.9 m^3, whereas, for light vehicles, it is possible to refuel 30 vehicles with a total volume of 22.9 m^3. Based on capital expenditure, the most representative capital costs are the production equipment (30%), high-pressure storage unit (20%) and the hydrogen compression system (18%).

Keywords:

Hydrogen; H_2 Refuelling protocols; Light and heavy vehicles; Numerical Optimization; CAPEX.

1. Introduction

Hydrogen as an energy carrier is currently seen as one of the most favourable ways to accelerate the decarbonization of various industrial sectors and vehicular mobility [1]. According to Perna et al [2], currently, there are approximately 200 hydrogen refuelling stations, mostly located in Japan, Germany, and USA. Yet, more than 5000 new stations are planned to be constructed by 2030.

Hydrogen-based refuelling stations comprise mainly four main steps, namely, production, storage, safety and utilization [3]. The selection of hydrogen production via requires considerable resources and their use, technological availability, efficiency, costs, environmental impacts and system integration options [4]. After production, the hydrogen needs to be stored [5]. According to the literature [4–9], storage and transport are the most difficult phases of the hydrogen supply chain. In order to use hydrogen as fuel, its physical state has to be altered in order to improve its density. Being hydrogen an energy vector that can be produced in a clean and environmentally friendly way, this gas is generally stored for local consumption or for transportation to the point of final consumption [3]. Either way, each solution must be studied individually in order to meet the specific needs. According to Demir and Dincer [8], identifying cost-effective pathways for supplying hydrogen remains an appealing prospect.

https://doi.org/10.52202/069564-0090

Refuelling gaseous hydrogen is a process that comprises two main ways: either the hydrogen is directly compressed in a tank using a compressor or the hydrogen is moved from a tank with higher pressure to the target tank at lower pressure [10]. In the context of vehicle refuelling stations, the storage of hydrogen in a gaseous state remains the most viable option [11]. Compressed hydrogen is a highly efficient methodology for hydrogen storage, but it requires the use of high-pressure systems. This represents an important issue because the energy density of the gas varies with the pressure inside the container. The fatigue caused by the repetitive cycles of high to low pressure, as well as, the inherent risks in having a pressurized gas are a key aspect in sizing the storage system [6,9,12].

For vehicular applications, it is required to have high-density storage systems, low weight and low cost, that are suitable for the hydrogen delivery system. High-pressure hydrogen storage technology is usually applied at hydrogen refuelling stations and hydrogen vehicles. The majority of refuelling stations require most of the following components: (i) hydrogen production equipment with a purification unit to secure that hydrogen purity meets the standards for supplying fuel cells; (ii) hydrogen compression system for high-pressure storage inside the station's main tanks; (iii) hydrogen storage tanks for either compressed gas or liquid hydrogen; (iv) equipment able to regulate pressure to 350 bar or 700 bar during the refuelling procedure; (v) a cooling unit to reduce hydrogen gas temperature down to − 40 °C to guarantee that during fast refills the vehicle's hydrogen tank does not exceed 85 °C, mostly to ensure the station safety; (vi) dispensers used to fill the vehicles tanks from the station's compressed storage containers; (vii) electrical and mechanical equipment such as valves, piping, pressure relief valves and hydrogen sensors [13].

Refuelling stations are categorized into off-site hydrogen stations and on-site infrastructures. The first type includes all the stations where hydrogen is delivered from a central production plant, being transported through pipelines or by heavy-duty trucks where hydrogen is stored in tube trailers as compressed gas [14]. For on-site stations, the hydrogen used to refuel the vehicles is generated locally. This represents a technical limitation because the station efficiency depends on the output quantity of the hydrogen generators, which typically ranges from 100 kg/day to 1000 kg/day. From an economic perspective, on-site hydrogen refuelling stations have a significantly higher capital investment cost due to the hydrogen production components, especially, on-site water electrolysis production. According to Perna et al [2], the investment cost of on-site stations may represent a capital cost 1.5 times higher than similar off-site stations with the same capacity.

Several authors are focused on studying the technical aspects of refuelling station operation. Miguel et al [15] showed with their experimental studies that the maximum gas temperature reached at the end of the filling increases linearly with the increase of the initial temperature while the temperature increase and the state of charge decreases linearly with increasing initial temperature. Zhao et al. [16] have developed numerical simulations, to identify the temperature increase within the hydrogen vehicle tank during the refuelling process at 350 bar (i.e., the so called H35 refuelling at 35 MPa). A similar study was performed by Wang et al [17] for fast filling at 700 bar (i.e., the so called H70 refuelling at 70 MPa). Maus et al [18] investigated the filling procedure taking into account tank systems with different storage volumes, from 2 kg to 10 kg hydrogen.

Some studies have been presented in the literature regarding the modelling of hydrogen refuelling station. These are mostly focused on thermodynamic models based on on-site electrolysis looking for energy-efficient station configurations, off-site production systems and respective delivery supply chain, and the definition of refuelling network location with or without production method [1,19–21]. However, these studies do not apply optimization algorithms in the design of the station operating conditions. Moreover, the focus is on finding the most economical design and not purely on energy efficiency. Also, it is important to notice that the current network park of refuelling stations for hydrogen vehicles is in its early stages. Thus, the refuelling infrastructure must be cost-effective in order to achieve successful market growth. The present work aims to contribute to the appeal of new mobility solutions.

The main purpose of this paper is to define a numerical optimization model for a hydrogen refuelling station for light and heavy vehicles. The station should include a hydrogen production unit, an electrolyzer and a system able to store hydrogen at high-pressure to later feed the compression cascade. The model considers the hydrogen properties and the physical constrain to size a hydrogen refuelling station, prior to its construction. It was defined as the objective function the minimization of the total storage volume, taking into account the expected number of vehicles to be fuelled.

2. Vehicle hydrogen refuelling

The process of vehicle refuelling with compressed hydrogen is subjected to control requirements in order to ensure that the vehicle tank is within a specified operating condition defined by an upper limit on pressure, and an upper and lower limit on temperature [19]. Thus, refuelling protocols have been established to define specific conditions for sizing hydrogen refuelling stations. In this section, SAE supply protocols are presented and discussed in order to understand the main constraints in the design of hydrogen refuelling stations.

https://doi.org/10.52202/069564-0090

2.1. Refuelling protocols

The hydrogen filling of light and heavy vehicles has been studied, improved, simulated and standardized by the Society of Automotive Engineers (SAE) since 2010. The purpose of defining these refuelling protocols is to ensure that this process is safe and that it maximizes supply performance. The first refuelling protocol, TIR J2601, was published in 2010, defining the standard for light-duty gaseous hydrogen surface vehicles [22].

Afterwards, in 2014 after a period of development with simulations and field tests, new versions were published: “J2601-2 – Refuelling Protocol for Gaseous Hydrogen Powered Heavy Duty Vehicles” and “J2601-3 – Refuelling Protocol for Gaseous Hydrogen Powered Industrial Trucks”. More recently, in 2020, a new version of TIR J2601 allowed modifying the protocols to facilitate the supply of H70 (hydrogen at 70 MPa for light cars) in tanks with a capacity of over 10 kg of hydrogen. Figure 1 presents the evolution of SAE supply protocols over the years [23].

This protocol determines the conditions under which the vehicle storage tank and dispenser should operate. The dispenser is connected to a high-pressure storage unit that ensures the pressure range required for refuelling. The supply pressure depends on three factors, namely, the ambient temperature, the precooling temperature of the hydrogen in the dispenser, the vehicle's tank volume and the respective initial pressure. During the refuelling process, the initial tank pressure should be 5 bar and the vehicle's Nominal Working Pressure (NPW) is defined as 35 MPa for heavy vehicles and 70 MPa for light vehicles). The mass flow rate of hydrogen to be supplied cannot exceed 60 g/s. Also, the hydrogen temperature limits vary between - 40 ºC and 85 ºC [22,24].

As stated, the NPW for light and heavy vehicles is different. For light vehicles, it is necessary to increase the pressure at which the gas is stored in order to increase the mass available in the system. As compression increases the temperature, when refuelling light vehicles, it is necessary to include a chiller in the station so the maximum admissible temperature in the tank at a pressure of 700 bar is not exceeded. In contrast to light vehicles, heavy vehicles have tanks with higher storage capacity, allowing these vehicles to be refilled with 35 kg of hydrogen at 35 MPa [22].

Thus, the expected performance for the protocol aims to guarantee a refuelling with a duration in the range of 3 minutes at a station, capable of pre-cooling the hydrogen to - 40 ºC. These conditions allow reaching a state of supply between 90 and 100% of the vehicle's capacity for NPW conditions and considering an ambient temperature of 15 ºC [19].

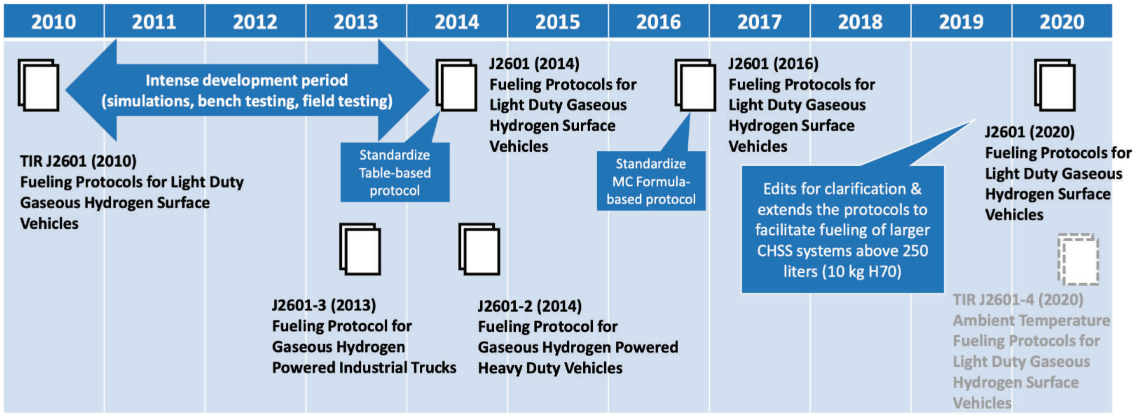

Figure. 1. Identification of SAE supply protocols between 2010 and 2020. The protocol J2601 determines the conditions under which the vehicle storage system and dispenser should operate. Adapted from [24].

The SAE J2601 protocol includes three main phases: (1) startup point; (2) refuelling phase; and (3) refuelling termination. In the first stage, it is ensured a secure connection between the dispenser nozzle and the vehicle. As soon as the connection is established, a signal is sent to verify that there is no error in the connection. Then, a pressure signal is sent to the tank to set the initial refuelling pressure and the second one to detect possible leaks and estimate the tank volume (estimated with an error of +/- 15%). During this phase, the hydrogen mass transfer limit to the tank is 200 g. Knowing the ambient temperature, the initial tank pressure, the refuelling temperature and the dispenser condition (hot or cold), the Average Pressure Ramp Rate (APRR) corresponding to the measured data is selected and the refuelling pressure condition is calculated. The initial phase is concluded when the mass of hydrogen begins to be transferred into the vehicle's tank. This is followed by the second phase, the main refuelling, in which the pre-cooling temperature is monitored during the refuelling and according to the calculated APRR. The temperature of the hydrogen when filling a tank needs to be monitored to ensure the safety of the process and to avoid overheating.

The validation of this process is based on the guarantee that the pre-cooling temperature is achieved. Otherwise, a process called Fallback Pressure Ramp Ratio (FPRR) is initiated and a new APRR is calculated. From the moment the refuelling process starts, the station controls the pressures at which the dispenser is delivering hydrogen. When the pressure in the dispenser reaches the limit established as the termination pressure, the refuelling process is complete [25].

Two main methods are used to implement SAE J2601 protocol: the LookUp Table method and the MC Formula. The LookUp Table method controls the evolution of the hydrogen pressure during the refuelling process based on the pressure and temperature in the vehicle's tank. It uses standardized table values, that specify pressure increases taking into account: vehicle tank capacity; type of refuelling system; hydrogen temperature when refuelling (T40, T30 and T20, i.e., the refuelling temperature of – 40 ºC, – 30 ºC, – 20 ºC, respectively); refuelling pressure (H35 or H70); type of vehicle-station interface and the hydrogen temperature at the dispenser outlet [22,26].

The method is based on the three identified phases of SAE J2601 protocol through the calculation of an APRR for a specific condition of ambient temperature and initial tank pressure.

The MC Formula is an alternative method based on a version of Honda's MC method that consists of analytical calculations. It uses thermodynamic properties to dynamically determine the APRR that controls the refuelling flow [10]. The MC formula can be illustrated in Figure 2, where all the parameters are presented. This method is defined for SAE J2601 boundary conditions and the APRR is adjusted according to the temperature measured at the dispenser outlet. It uses empirical equations whose coefficients are determined through the initial tank pressure, ambient temperature and tank capacity, constantly calculating the filling pressure throughout the filling.

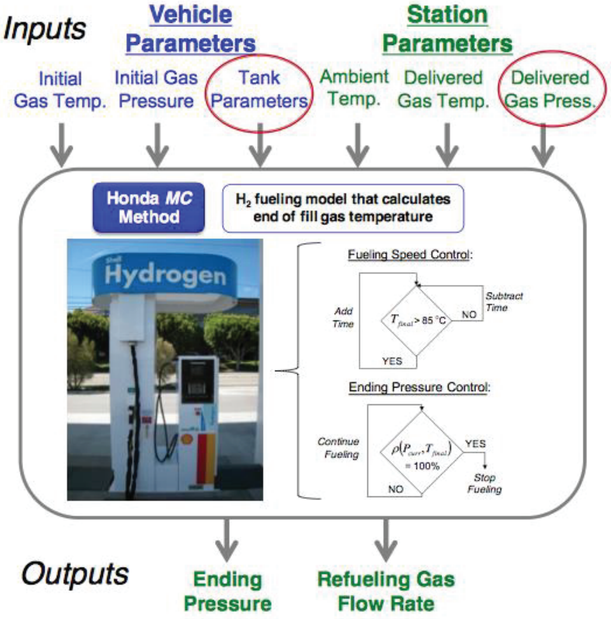

Figure. 2. Diagram control for MC formula method implementation considering the SAE J2601 protocol requirements. Adapted from [10,22].

Similarly to the LookUp Table method, the MC Formula is based in three phases. In the refuelling phase, the formula MC measures and actively uses the precooling temperature in the dispenser to calculate the hydrogen Mass Average Temperature (MAT) and the mass average enthalpy used to decide the APRR and termination pressure during the refuelling [27,28]. The refuelling process is controlled by both APRR and target pressure. The APRR is calculated based on the mass flow rate and pre-cooling temperature measured at the dispenser outlet. The actual pre-cooling temperature at the dispenser is calculated, as well as, the time defined as the total period needed to fill the vehicle tank, varying from a minimum to a maximum pressure [22]. The MC Formula method uses a MAT based on the pre-cooling temperature measured after thirty second (MAT30) to control the process until the transition pressure is reached. It is important to mention that both LookUp Table and MC formula methos apply the same boundary conditions and both collect information from the station to complete the refuelling safely.

2.2. Hydrogen Refuelling Constraints

As previously stated, the hydrogen refuelling station needs a hydrogen production equipment, a system able to store hydrogen to later feed the compression system, a chiller and a dispenser. Thus, the refuelling station operation is based on six main steps [20]:

- Step 1 – Hydrogen in gaseous state is produced through the water electrolysis in the electrolyzer which is stored at low pressure;
- Step 2 – A buffer is used to storage the hydrogen at low pressure to accumulate the required mass of hydrogen to start the compression;
- Step 3 – Hydrogen is admitted into the compression unit, able to pressurize the gas up to 10 times higher than the inlet condition;
- Step 4 – Hydrogen is stored at high pressure in containers after its compression in the gas cascade system;
- Step 5 (mandatory only for H70) – A chiller is used for hydrogen cooling till it reaches the required temperature;
- Step 6 – Hydrogen is filled through a dispenser connected to the vehicle's nozzle.

One of the main operational constraints of a refuelling stations is related with the hydrogen compression. Hydrogen rapid compression leads to the temperature increase inside the tank which, in case of an exaggerated increase, can compromise the complete refuelling station [9]. As previously mentioned, to prevent this event, the maximum temperature limit inside the tank was set at 85 ºC. In addition to safety considerations, this limitation is imposed because the density of the gas changes with the temperature, and, consequently, the existing mass inside the tank decreases with the temperature, affecting the State of Charge (SOC). A SOC close to 100% means that the refuelling allowed filling the tank with the highest mass capacity of hydrogen possible, maximizing the vehicle's autonomy. The technological solution to control this problem is cooling of hydrogen, incorporating a chiller in the refuelling system [10].

As the chiller represents an additional investment cost, the hydrogen refuelling mass flow rates must first be set, which should be lower than 60 grams of hydrogen per second for H70 and 120 grams of hydrogen per second for H35 (SAE J2601).

Regarding safety, ISO 19880 [29] defines some conditions that must be fulfilled so the refuelling station could operate. The refuelling stations must be designed to minimize gas leaks during station operation. Closing valves should be incorporated to minimize the risks in the event of a hydrogen leak. Regarding storage, containers must be equipped with valves activated by pressure or temperature. All materials must be compatible with hydrogen at the operating temperatures and pressures. Materials should be selected according to ISO 15916, ISO 11114 and ISO 16573.

3. Refuelling station modelling

The aim of this study is to define a mathematical model for the design of a hydrogen refuelling station for light and heavy vehicles. Thus, a case study was defined to model a real problem regarding the refuelling requirements for H35 and H70 and considering tangible operational parameters explained in this section.

3.1. Description of refuelling station

The refuelling station under modelling (Figure 3) must be able to supply 300 kg of hydrogen per day. The system needs to include the production equipment, an electrolyser, which feeds a low-pressure storage buffer tank at 35 bar. The compressors aim to raise the pressure to a maximum of 500 bar and store the hydrogen in high-pressure containers arranged in a cascade system, in order to minimize their energy consumption. The hydrogen is stored in skids with several containers connected to a certain pressure. Note that a pressure cascade storage system is considered in order to prevent multiple fatigue cycles that the skid containers are subjected from successive hydrogen filling processes. For cascade storage system, when the fuelling is initiated, the hydrogen pressure in the vehicle tank is compared with the tank pressure value, level by level till the final pressure and mass are reached. When the refuelling process is complete, the storage is refilled, starting by the lowest pressure level [12,19].

The mass of hydrogen is supplied through a dispenser from the high-pressure storage system, depending on the pressure level. A very important requirement that defines a large part of the problem is related to the need in guaranteeing a pressure differential of 50 bar between the vehicle tank and the stored hydrogen so the refuelling process can be validated.

https://doi.org/10.52202/069564-0090

In the case of refuelling heavy vehicles (buses), hydrogen is supplied directly from storage unit at 500 bar to the dispenser. In case of refuelling light vehicles, hydrogen stored at 500 bar is compressed to a second storing level, till reaching a pressure of 900 bar. Thus, to proper sizing the refuelling station, it is necessary to stablish the number of vehicles to fill, calculate the required mass of hydrogen, define the number of pressure levels and minimum hydrogen volumes to store at each pressure level. For this study it was assumed that the refuelling station should be able to:

1. Supply 10 heavy vehicles at 350 bar (H35), considering 2 skid pressure levels. This solution allows refuelling hydrogen at a maximum of 120 g/s, in order to comply with the maximum required refuelling time of 15 minutes. It is assumed that a mass of 30 kg is supplied by the dispenser. It is also assumed that the vehicle arrives at the station with the minimum hydrogen mass of 6 kg at 50 bar.
2. Supply 30 light vehicles at 700 bar (H70), considering 3 skid pressure levels. During the refuelling process is theoretically expected to dispense 4.2 kg.

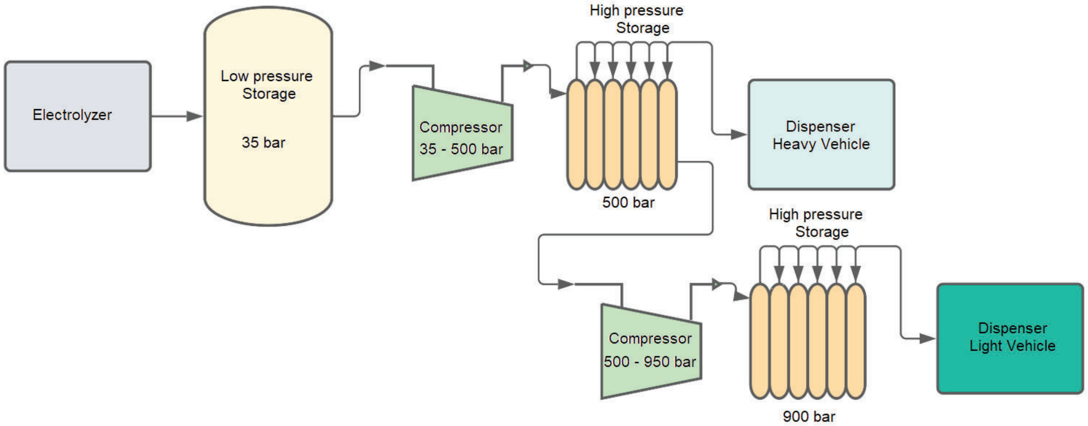

Figure. 3. Schematic representation of the hydrogen refuelling station considering the compression levels and the low and high-pressure storage.

3.2. Mathematical modelling

The model formulation includes the definition of the objective function, decision variables and physical constraints, for which an optimization algorithm is applied in order to disclose the best solution domain. Thus, at each complete simulation, the implemented model runs, iteratively, all the routines of the physical model [30].

3.2.1. Objective function

The mathematical model for storage sizing and refuelling is based on several physical variables, such as the storage volume (v), the pressure at which the hydrogen is stored (p) and the mass of hydrogen filled (m).

The objective function of the mathematical model is to minimize the total volume of high-pressure storage, whereas, the volume can be calculated through the hydrogen density. Thus, the objective function is defined by equation (1).

$$\begin{gathered} min \quad v \\ where \quad v = \frac{m}{Fp^2 + Gp + H} \end{gathered} \tag{1}$$

In equation (1), terms F, G and H correspond to the coefficients from the function of the density variation of hydrogen. The determination of these coefficients is based on the numerical approximation through *Polyfit* routine at Matlab®, considering reference discrete values that relates the density of hydrogen with the pressure for an operating temperature of 25ºC. The 2nd degree polynomial is presented in equation (2).

$$\frac{m}{v} = -2.55\times10^{-2}\,p^2 + 7.39\times10^{-2}\,p + 3.64\times10^{-1} \quad [\mathrm{kg/\,m^3}] \tag{2}$$

3.2.2. Decision variables and constraints

Defining the decision variables is in fact one of the hardest and/or most crucial steps in formulating an optimization problem. Three types of physical quantities were defined as explicit decision variables for the numerical model. For all of them upper and lower bounds were set in order to establish the operational relationships. The bounds in the variables guarantee that the optimum solution is within the technical operating capability. One of the main decision variables is the pressure at which the hydrogen is stored in the high-pressure system. The lower and upper pressure limits for each skid level are based on values that take into account the components to be used in the station and its operating requirements. Table 1 presents the pressures limits for both light and heavy refuelling models. For both H35 and H70 refuelling, it is defined a minimum pressure of 100 bar on skid 1. The lower pressure limit at each skid corresponds to the maximum value obtained by the optimization model at the previous skid pressure level. Thus, the hydrogen pressure at skid 1 ($p_{H35,1}$ and $p_{H70,1}$) varies between 100 and 375 bar.

The pressure in the skid 2 ($p_{H35,2}$ and $p_{H70,2}$) cannot exceed a maximum pressure of 500 bar. For H70 refuelling, a third skid level was considered ($p_{H70,3}$), establishing an upper limit of 900 bar.

Table 1. Lower and upper limits for skid pressure

Type of vehicle	Skid level	Variables and respective limits [bar]	
Heavy vehicles (H35)	Skid 1	$100 \leq p_{H35,1} < 375$	(3)
	Skid 2	$p_{H35,max,1} \leq p_{H35,2} \leq 500$	(4)
Light vehicles (H70)	Skid 1	$100 \leq p_{H70,1} < 375$	(5)
	Skid 2	$p_{H70,max,1} \leq p_{H70,2} < 500$	(6)
	Skid 3	$p_{H70,max,2} \leq p_{H70,3} \leq 900$	(7)

The second decision variable is the volume of hydrogen stored at each skid level, $v_{H35,1}, v_{H35,2}$ for H35 refuelling and $v_{H70,1}, v_{H70,2}, v_{H70,3}$ in the case of H70 refuelling. Due to operational considerations, it was set that the volume stored at high-ranked skids with pressure levels (see equation (8) and equation (9)).

$$v_{H35,1} \leq v_{H35,2} \quad [\mathrm{m}^3] \tag{8}$$

$$v_{H70,1} \leq v_{H70,2} \leq v_{H70,3} \quad [\mathrm{m}^3] \tag{9}$$

The third decision variable is the mass of hydrogen transferred from the skid to the vehicle during the refuelling ($m_{H_2 out,x}$). At each filling, there is a quantity of mass provided by the skid, depending on the final mass that is required to complete each refuelling. Yet, the mass that is supplied in the first H35 filling by the first pressure level must be lower or equal to 30 kg (equation (10)).

$$m_{H_2 out,1} \leq 30 \quad [\mathrm{kg}] \tag{10}$$

For all refuelling processes, the pressure drop of 50 bar between the station skid and the vehicle tank must be guaranteed (equation (11)).

$$p_{skid} - p_{\text{vehicle tank}} \geq 50 \quad [\mathrm{bar}] \tag{11}$$

3.2.3. Optimization method

In order to implement the optimization problem, the *MS Excel® Solver* was used, considering the Generalized Reduced Gradient (GRG) method. This popular optimization method is able to solve nonlinear optimization problems, only requiring that the objective function is differentiable. This method allows to solve the nonlinear problem dealing with active inequalities. The variables are separated into a set of basic (dependent) variables and non-basic (independent) variables. Then, the reduced gradient is computed in order to find the minimum in the search direction. This process is repeated until the convergence is obtained.

The used solver includes a multi start method that can improve the prospects of finding a globally optimal solution for an optimization problem [31,32].

4. Results and discussion

After defining the decision variables, their maximum and minimum limits, as well as the problem constraints, the mathematical model was programmed and the results obtained are presented in this section. The simulation results are depicted for heavy and light vehicles. The optimal values of pressure at each storage skid, the skid storage volumes and the hydrogen mass that is provided at each fuelling are presented considering the minimum storage capacity required.

4.1. Refuelling of heavy vehicles

The value of the objective function - minimize the total storage volume – corresponded to a storage volume of 36.90 m^3, being obtained a volume of 10.58 m^3 in the first skid and 26.32 m^3 in the second skid. The total stored volume can be considered high, since it represents a large volume to physically store, assuming normal conditions of pressure and temperature.

According to the results (Table 2), the pressures in the high-pressure storage system fulfil the functional requirements defined by equations (3) and (4). The pressure in the first skid does not exceed 375 bar and in the second level does not exceed 500 bar.

Table 2. Optimal solution for heavy vehicles refuelling (H35)

Parameter	Variable	Value
Volume [m^3]	Total volume, v	36.90
	Skid 1, $v_{H35,1}$	10.58
	Skid 2, $v_{H35,2}$	26.32
Pressure [bar]	Skid 1, $p_{H35,1}$	128.6
	Skid 2, $p_{H35,2}$	395.6

Figure 4 presents the mass of hydrogen dispensed at each skid ($m_{H_2\,out,x}$). As the number of fillings increase, the mass of hydrogen to be dispensed from the skid 1 decreases. This decrease is compensated by the raising mass provided skid 2. By the end of the 6th refuelling, it is observed that the mass provided by both skids is similar. This outcome is related to the fact that the initial pressure at which the hydrogen is stored in the skid 1 is very close to the supply pressure, which means that the useful mass in that first level is smaller than the useful mass available in the second. Also, it is shown that the first refuelling provides a mass lower than the required 30 kg.

Figure 5 shows the pressure drop between the heavy vehicle tank and the storage containers. It appears that the pressure decreases as fillings are accomplished, since the decrease in the usable available mass of hydrogen results in a decrease of the pressure in storage.

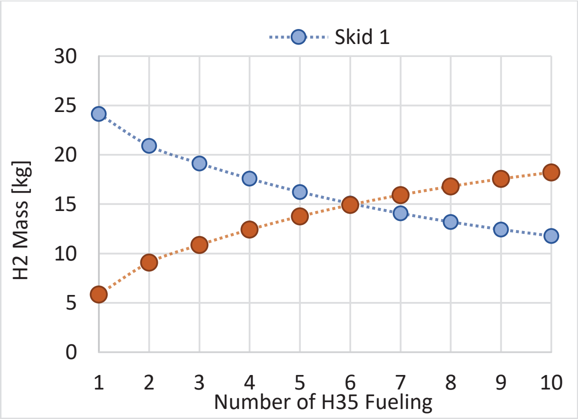

Figure. 4. Mass of hydrogen dispensed at each skid level for H35 refuelling.

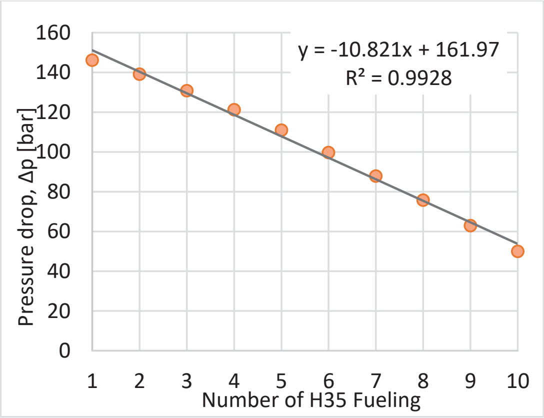

Figure. 5. Evolution of pressure drop between the station skid and the vehicle tank for H35 refuelling.

4.2. Refuelling of light vehicles

Regarding the light vehicles, the results for the total storage volume and the respective skid values are presented in Table 3. The total volume corresponded to 22.89 m^3, being obtained an equal volume of 7.63 m^3 for all 3 skids. Taking into account the number of vehicles to be fuelled and the pressure required by the system, these values are acceptable and allow all vehicles to be filled with the expected 4.70 kg of hydrogen. Thus, in order to respect all problem constraints, it is necessary a 5 hours period to fuel the 30 light vehicles.

The pressure in skid 1 and skid 2 corresponds to the lower limit established as the boundary condition, a value of 100 bar and 375 bar, respectively. In the skid 3, the pressure reaches the value of 750 bar. The value of the maximum pressure of the storage system is, in theory, the most limiting input parameter, but also the most important one in the sizing of the filling station. It is estimated that changing this input will cause sudden changes in the total volume required for hydrogen storage. Consequently, larger volumes of storage required imply a greater initial investment in the construction of the station.

Table 3. Optimal solution for light vehicles refuelling (H70)

Parameter	Variable	Value
Volume [m^3]	Total volume, v	22. 9
	Skid 1, $v_{H70,1}$	7.63
	Skid 2, $v_{H70,2}$	7.63
	Skid 3, $v_{H70,3}$	7.63
Pressure [bar]	Skid 1, $p_{H70,1}$	100
	Skid 2, $p_{H70,2}$	375
	Skid 3, $p_{H70,3}$	750

Figure 6 presents the mass of hydrogen dispensed at each skid ($m_{H_2\,out,x}$) considering the refuelling time. Equally to the results obtained for heavy vehicles, as the number of fillings increase, the mass of hydrogen to be dispensed from the skid 1 decreases. This decrease is compensated by the raising mass provided by both skid 2 and skid 3. In the skid 3, where the hydrogen storage pressure is higher than the final pressure in the vehicle tank ($p_{\text{vehicle tank}} = 671.4 \text{ bar}$), the results show that in the last hour of refuelling, almost 50% of the total mass of the vehicle's tank comes from the skid 3, taking into account that the two skids lose their ability to respond as fillings occur. Figure 7 shows the pressure drop between the light vehicle tank and the storage containers. As the refuelling is completed, the pressure differential decreases.

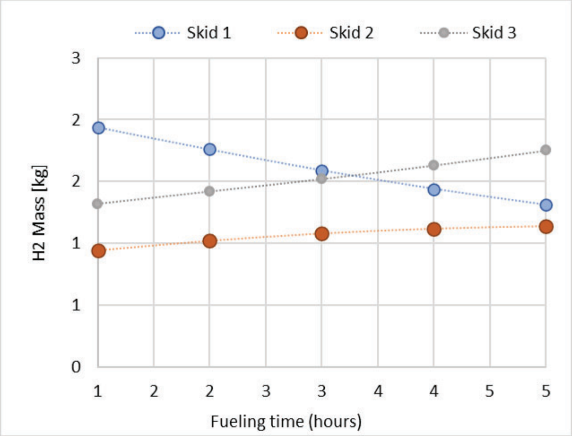

Figure. 6. Mass of hydrogen dispensed at each skid level for H70 refuelling.

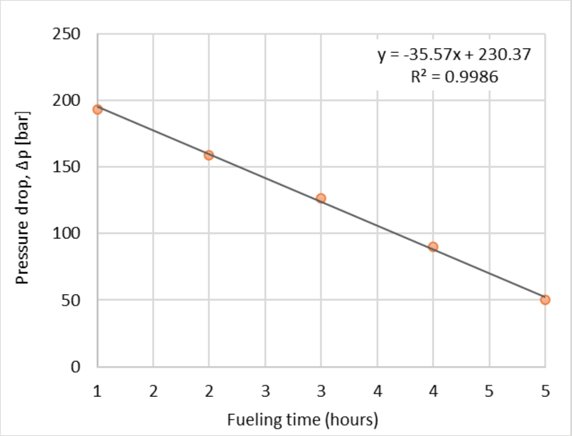

Figure. 7. Evolution of pressure drop between the station skid and the vehicle tank for H70 refuelling.

4.3. CAPEX determination

The costs of a hydrogen refuelling station depend on the characteristics of the equipment and components. Considering the components that the hydrogen refuelling station, the total investment cost can be determined by market sourcing of components with the characteristics closest to those obtained from the optimal solution. When determining the total capital costs, in addition to all the components already identified, it is necessary to calculate all accessories and labour costs.

The CAPital EXpenditure – CAPEX – is the total amount invested in the project [33]. Considering the data collected from the market, it was possible to estimate the relative weight of each component of the hydrogen refuelling station. Based in Figure 8, the highest percentages are represented by the cost of production equipment (30%), high-pressure storage unit (20%) and the hydrogen compression system (18%).

When sizing a hydrogen refuelling station, the electrolyzer and the compressors are components with more standardized working characteristics and their capital costs do not vary significantly with the increase in installed capacity. However, high-pressure storage unit cost depends on the capacity required for a given filling frequency, which in turn depends on the total volume and daily hydrogen requirements. The analysis also shows that the hydrogen dispenser only represents 7% of the total capital costs.

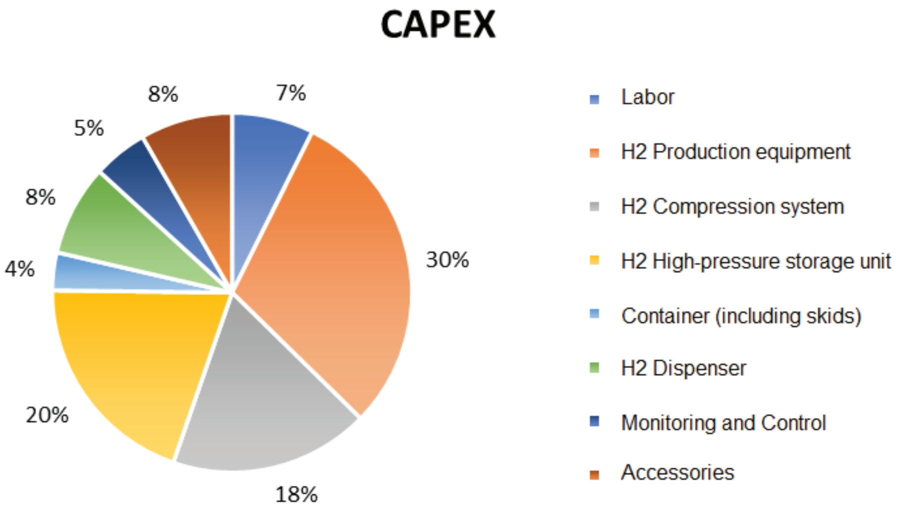

Figure. 8. CAPEX for the hydrogen refuelling station considering the commercial options for the optimal solution disclosed by the numerical model.

5. Conclusions

This paper aims to define a numerical optimization model for a hydrogen refuelling station to supply both light and heavy vehicles. The objective function is to minimize the total storage volume, taking into account the number of vehicles to be refuelled. The process of vehicle refuelling with compressed hydrogen was subjected to control requirements to ensure that the vehicle tank is within a specified operating condition defined by an upper limit on pressure, and an upper and lower limit on temperature. The

The refuelling station was defined considering the electrolyzer, a low-pressure storage buffer, the compressors aim to raise the pressure and the hydrogen high-pressure containers arranged in a cascade system in order to minimize their energy consumption. The hydrogen is stored in skids with several containers connected to a certain pressure. The station should be able to supply light and heavy (buses) vehicles. Thus, theoretically, the on-site infrastructure, 10 heavy vehicles at 350 bar and 30 light vehicles at 700 bar should be supplied. For H35 fuelling, 2 skid pressure levels were considered, allowing two fillings per hour. In this case, it is assumed that a mass of 30 kg is supplied by the dispenser. The compression cascade for light vehicles considers 3 skid pressure levels and is expected to dispense 4.2 kg. The objective function is to minimize the total storage volume required. As decision variables, the pressure at each storage skid is considered, as well as the hydrogen mass dispensed to the vehicle tank. One of the most important constraints is the pressure differential of 50 bar between the high-pressure skid and the vehicle tank that should be guaranteed at all vehicle fillings, so the refuelling can be validated. The requirements regarding the refuelling process in order to prevent over-heating and over-filling significantly influence hydrogen refuelling station design and have a strong impact on its performance.

Thus, the hydrogen filling of light and heavy vehicles has been studied and standardized by SAE through the implementation of fuelling protocols. According to the SAE J2601 protocol, the mass flow rate of hydrogen to be supplied cannot exceed 60 g/s. Also, the hydrogen temperature limits vary between - 40 ºC and 85 ºC.

Also, fast refuelling of hydrogen is constrained by the thermodynamic properties of hydrogen under compression. The optimization results show that is possible to refuel 10 heavy vehicles considering a total storage volume of 36.9 m^3, whereas, for light vehicles, it is possible to refuel 30 vehicles with a total volume of 22.9 m^3. Based on CAPEX, the most representative capital costs are: the production equipment (30%), high-pressure storage unit (20%) and the hydrogen compression system (18%).

In conclusion, the skid pressure, the useful mass of hydrogen and the storage volume are the most important parameters in the design of hydrogen refuelling station. Their variation can cause drastic changes in the capital investment cost to construct the station. As future work, it is proposed the development of a techno-economic model, considering the integration of costs in the process of optimizing the design of the on-site hydrogen refuelling station.

Acknowledgments

This work was supported by FCT - Portuguese foundation for science and technology through the R&D Units Project Scope UIDP/04077/2020 (METRICS) and R&D Unit Project Scope UIDB/00319/2020 (ALGORITMI).

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