Model of hydrogen production system for investigating the energy flexibility of residential buildings

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Model of hydrogen production system for investigating the energy flexibility of residential buildings

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Acknowledgements

After an intensive last year of Master, writing this acknowledgement note is the ultimate touch to my Master project. It has been a period of continuous learning. I would like to express my gratitude to all the people who, in a higher or smaller extent, have supported my scientific and cultural development.

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Alejandro Martínez Henríquez

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1. Introduction

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The world energy consumption increases every year (Figure 1.1). The energy consumption by sectors is represented in the Figure 1.2. As represented, the residential sector constitutes 27% of the total energy consumption in the world, after industry and transportation [1].
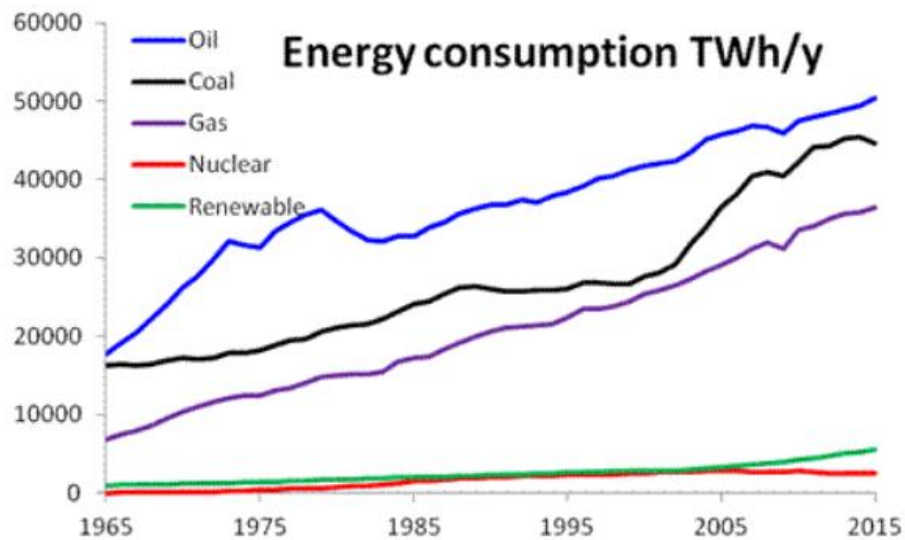
Figure 1.1: World Energy consumption [2].
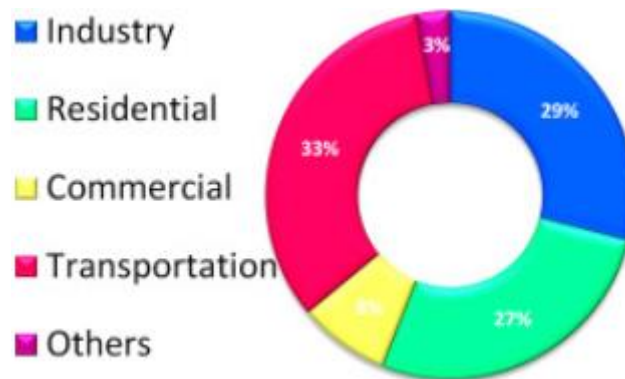
Figure 1.2: Sectorial shares of global energy consumption [1].

The increase of world energy consumption is reflected in the CO_2 print (as shown in Figure 1.3). The CO_2 is the result of the combustion of fossil fuels as oil, coal and natural gas, processes usually used for the generation of energy.

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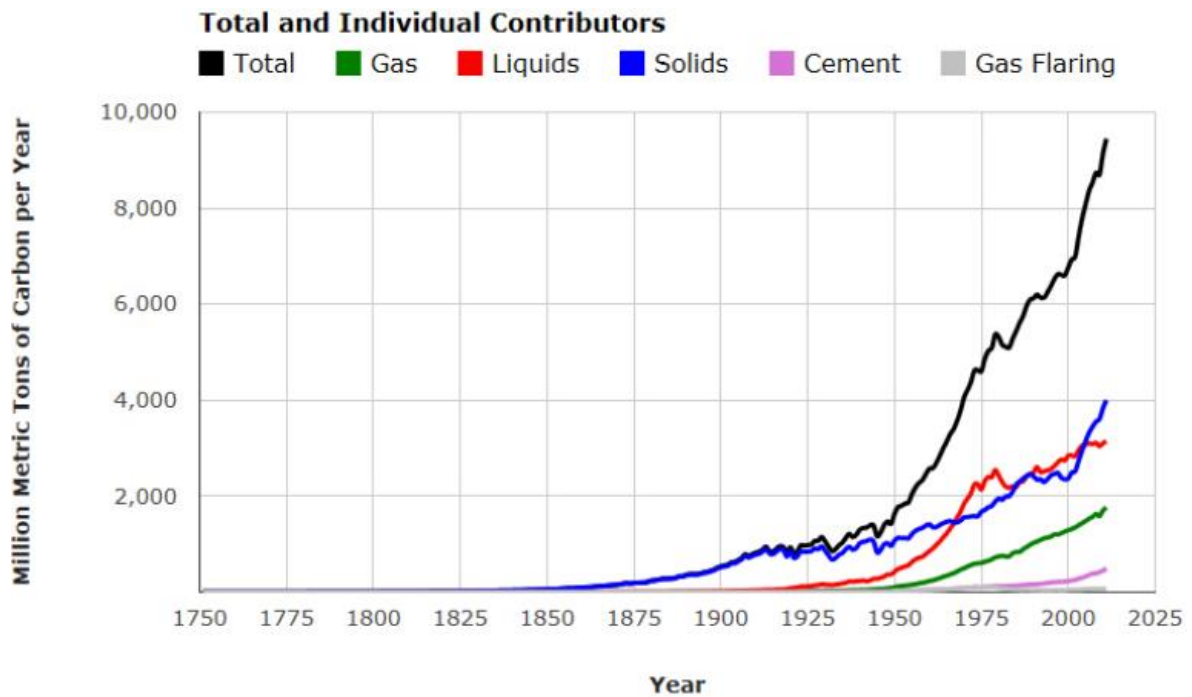
Figure 1.3: Annual Global Fossil-Fuel Carbon Emissions [3].

The CO_2 emissions have an important impact on global climate contributing to the greenhouse effect [4]. Therefore, there is an imperative need to reduce this CO_2 print. To achieve this goal various procedures are available.

One possibility could be to use fuels with less footprint emissions such as synthetic natural gas (SNG). The use of SNG could reduce the CO_2 emissions of approximately 45% compared to coal [5]. Another solution is to decrease the use of fossil fuels. This could be achieved by using renewable energy in a higher extent. However, the issue that could arise is the fact that this kind of energy is submitted to weather changings (speed of the wind, hours of sun…), so the amount of power obtained is not constant overtime. For example, the production of photovoltaic panels is much higher during summer than during the other seasons. Therefore, there is a discrepancy between the demand and the production of the energy required. A way to overcome this problem is to optimise a system for seasonal energy storage. This kind of system will allow the storage of the power generated by renewable sources (when these are working) and its consumption when required.

There are several ways to store the produced energy. One possibility is to store the energy in dams, they have a quick response, but the conditions required for their use

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are not easily encountered. Another solution would be to store a limited quantity of electrical energy in electrical batteries, for short periods of time. They have a good response, but the rate between the volume and the specific energy density is high, especially for Lead Acid and NI-Cd batteries as shown in Figure 1.4.
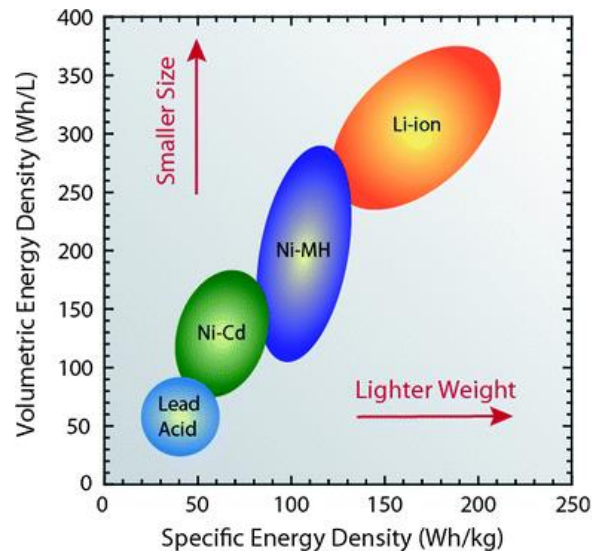
Figure 1.4: The battery comparison chart illustrates the volumetric and specific energy densities showing smaller sizes and lighter weight cells [6].

The technology of storage which use the electrical energy to produce hydrogen (H_2) is gaining increasing importance nowadays. One of the main reasons is the fact that hydrogen combustion does not generate CO_2 products. Another reason is the high specific energy density of H_2 (120000 kJ/kg). A comparison between hydrogen properties and other fuels properties is reported in the table 1.1. As shown, overall, hydrogen has the best performances compared to petrol and methane (diffusion coefficient in air, specific heat at constant pressure, etc).

Hydrogen used as energy vector is currently used in various countries and this technology is under constant development.

In Japan, a new Strategic Energy Plan (SEP) was formulated by the Government after the accident at Fukushima Daiichi Nuclear Power Station. The hydrogen and its utilization with fuel cells play a central role in the SEP. They are building a new system of hydrogen pipelines in order to install a Hydrogen Fuel Cell in every house and to use hydrogen as their principal energy vector [8].

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Table 1.1: Properties of some fuels (Petrol, Methane and Hydrogen) [7]

Property	Petrol	Methane	Hydrogen
Density [kg/m³]	4.40	0.65	0.084
Diffusion coefficient in air [cm²/s]	0.05	0.16	0.61
Specific heat at constant pressure [J/kg]	1.2	2.22	14.89
Flammability limits in air [% volume]	1.0 - 7.6	5.3 - 15.0	4.0 - 75.0
Auto-inflammation temperature [°C]	228 - 471	540	585
Flame temperature in air [°C]	2197	1875	2045
Theoretical explosion energy [kg_{TNT}/m^3_{gaz}]	2.02	7.03	44.22

China is also building a new economy plan focused on hydrogen technology. Their main objective is to reduce the coal-based energy system by replacing it with hydrogen technology to improve the energy security and to reduce greenhouse gas emissions [9].

Europe is also working on several projects aiming to achieve an optimal and efficient use of hydrogen as energy vector. Their goal is to use the fuel cell as energy convertor in 2020 [10]. In this context, is noteworthy to mention that BENELUX has one of the biggest hydrogen pipelines in the world [11].

Colruyt Group (in southwest of Brussels, Belgium) works on a project (Don Quichote project) which uses hydrogen as fuel for their machines. They store hydrogen created using green electricity produced by wind farms and solar panels. This hydrogen is used for transport and to produce electrical energy when the wind farm and solar panels don't produce all the energy required.

The hydrogen cannot be easily found in a significant quantity and the available hydrogen is generally combined with other elements, such as oxygen in water, carbon in hydrocarbons, and both in biomass. Hydrogen is a gas that must be produced. Currently, 60 million tons of hydrogen are generated per year and its consumption is growing 6% per year [12].

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In industry hydrogen is mainly used for the refinery of fossil oils (50%) and the synthesis of ammonia (34%). The rest of hydrogen (16%), is used for the synthesis of other chemicals or for energy production [13].

Nowadays, 96% of hydrogen is produced from fossil fuels and 4% from water electrolysis [14], because reforming of hydrocarbons is a well-understood industrial process and persist to be less expensive than water electrolysis [15].

This work will be focused on hydrogen obtention by water electrolysis in order to reduce the use of fossil fuels and to reduce the CO_2 footprint.

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2. Objective

The main goal of this project is to develop a reliable model of a building system able to investigate the energy flexibility of residential buildings which possess energy produced by renewable sources and a hydrogen-based energy storage system.

The system will include: the production of hydrogen by renewable sources as photovoltaic panels (PV) or wind turbines, the storage of the H_2 produced and the electricity produced using the H_2 in a fuel cell (FC) to fill electrical batteries. The programme that will be used to model is Modelica.

This work will serve to verify if the system realisation could be technically possible and that the seasonal storage can be executed. Economic study will not be made because nowadays this technology (at small scale as a building) is not already available in the market.

3.   State of the art of hydrogen-based energy storage systems

The system investigated in the thesis is composed of the followings subsystems:

- The energy source which can be integrated with a renewable energy source as PV panels, wind turbines, both or the energy mix of the country;
- The electromechanical part which is combined with a water electrolyser, a hydrogen Fuel Cell and one or more batteries;
- The mechanical part which can be composed of a water pump, a hydrogen compressor and an expander system (hydrogen expander and valve);
- The hydrogen storage is realized in one or more tanks of hydrogen;
- The building load which is defined by the electrical consumption, the heat demand of the building or both.

All these subsystems will be further detailed in the following subsections. A diagram of the system is represented in Figure 3.1.
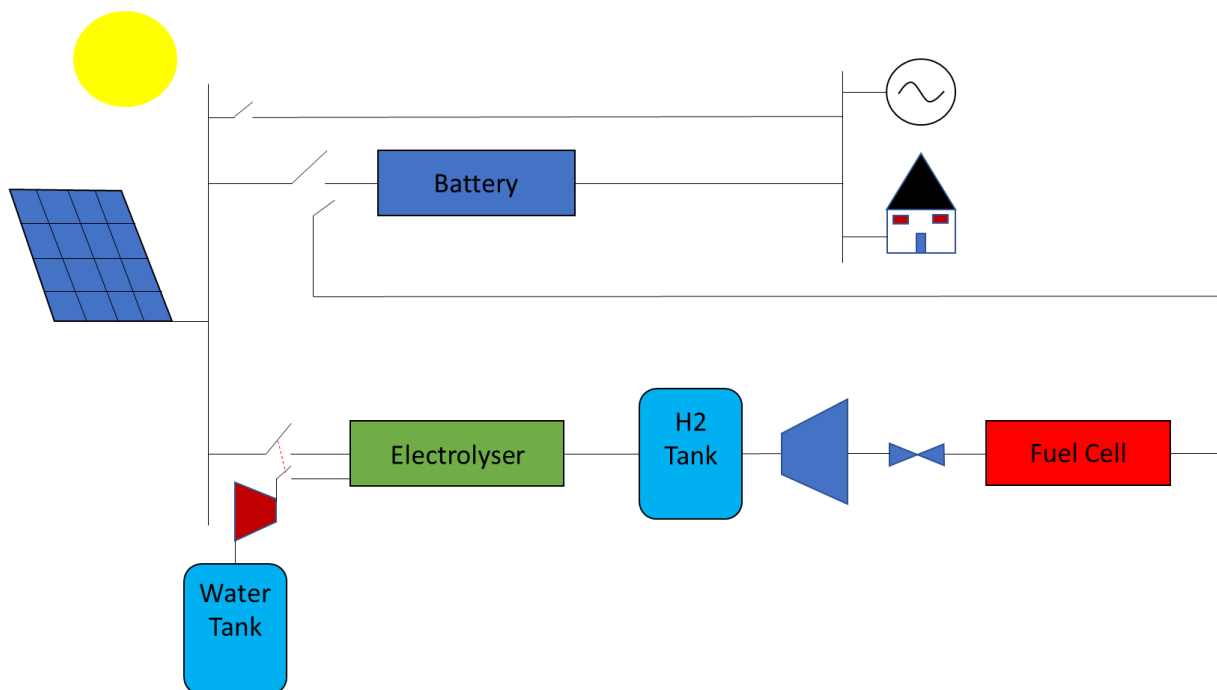
Figure 3.1: Schema of the studied system

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3.1. Energy sources

The energy source of the system depends on the conditions of the place where the system will be located. As explained before, renewable energy sources such as solar panels and wind turbines can be used to produce hydrogen in a green form (Colruyt Group). In this project, photovoltaic panels are chosen as principal source of renewable energy.

3.1.1. Photovoltaic panels

The photovoltaic panels (PV panels) are used around Europe as one of the most important renewable energy sources as can be observed in Figure 3.2. The mains advantages of PV panels are the easiness of installation, they require a low maintenance, the price is continuously decreasing and can be used almost anywhere there is sunlight [16]. However, the PV panels don't have a good electrical performance and they reach a maximum efficiency of 20 %. Moreover, their efficiency depends on the type of cells and the climatic conditions [17].
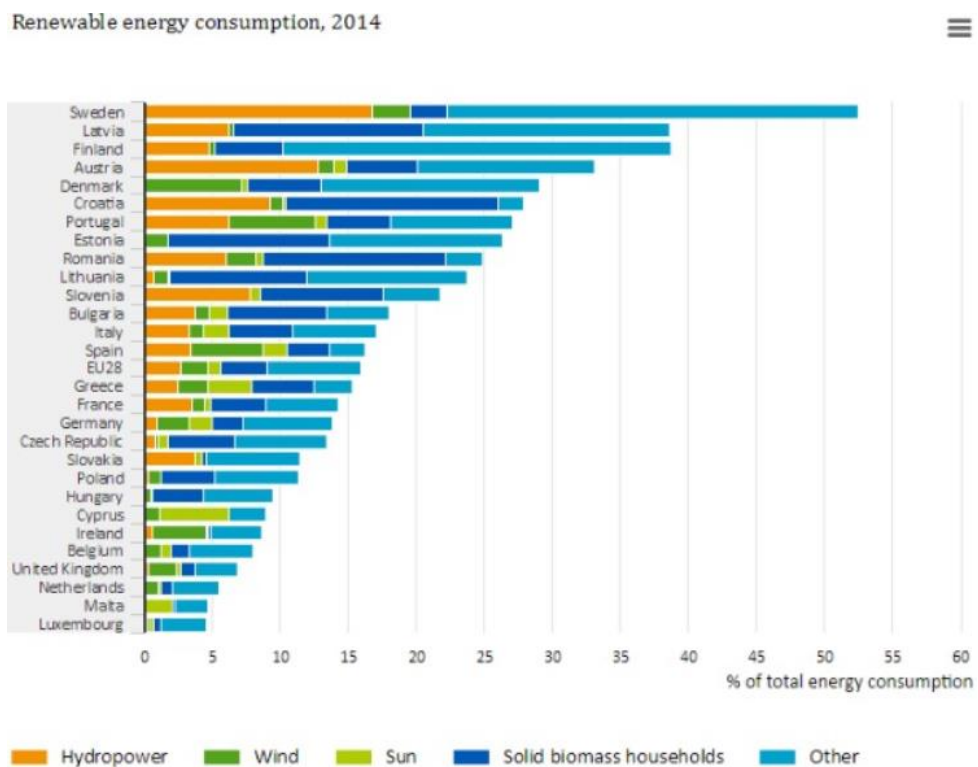
Figure 3.2: Renewable energy consumption in Europe [18].

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The photovoltaic panels are composed of materials that absorb the solar radiation in form of light and transform it into electrical power. There are different types of PV panels that have been used up to date. The most frequently used are the mono- and poly-crystalline PV panels which are made of silicon as the main material.

The solar irradiance (measured in W/m^2) is defined as the incident power per unit area received from the sun in form of electromagnetic radiation. The capture and harnessing of all the available irradiance strongly depends on the angle of incidence of the solar radiation. The maximal power is obtained when the incidence is normal to the surface.

The total energy obtained from sun radiation on the same surface (measured in kWh/m^2), place and moment is called, solar irradiation.

It is important to know what it is the real instantaneous power that arrives per m^2 to the photovoltaic panels and how much of it is transformed in electricity. For that, it is imperative to know some parameters, such as the angles between the sun and the PV panel (Figure 3.3), and the type of PV panel used.
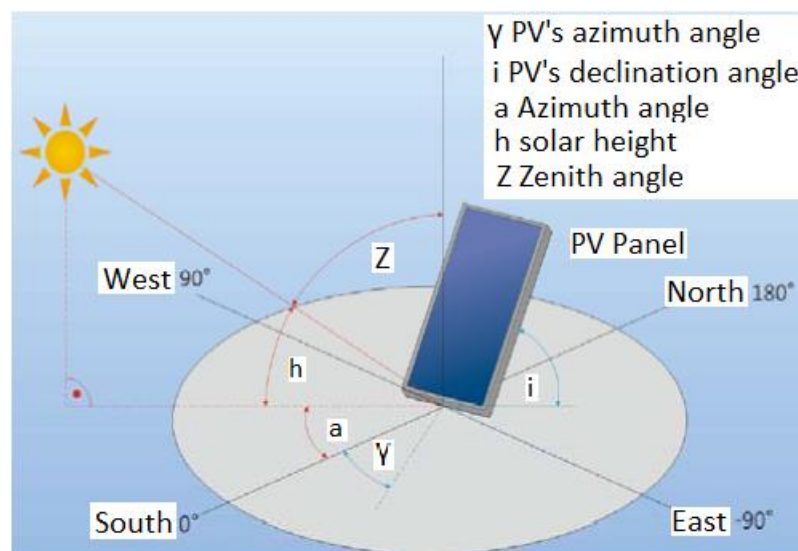
Figure 3.3: Representation of the angles between the PV panel, the Earth and the position of the sun.

The use of PV panels to produce the required energy for hydrogen generation in the electrolyser has been widely studied [19–21].

According to the above-mentioned information, an irradiation model and efficiency model will be made in the section 4.1. Therefore, the data of the irradiations has been taken for the city of Brussels and the characteristics of the PV panels chosen are presented on the **ANNEX**.

3.1.2. Energy mix

The energy mix is an assembly of different primary energy sources from which secondary energy, usually electricity, is produced. For each country it depends on [22]:

- The availability of usable resources;
- The quantity and the type of energy needed.
- Economic, demographic environmental and geopolitical factors.

In all systems connected to the grid, the energy mix is present in a smaller or bigger extent. The storage of hydrogen can produce benefits to the grid, as a damper for the balance.

If the energy obtained using PV panels is not sufficient to produce the energy required for the domestic consumption, it can be completed using the network (energy mix).

3.2. Electrochemical part of the system

This section focusses on the elements of the system on which electrochemical reactions are performed in order to transform the energy. These elements are the electrolyser, the fuel cell and the batteries. The system of energy storage is a hybrid system formed by batteries and hydrogen tanks. Electrical energy is obtained using the batteries and the fuel cell.

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3.2.1. Fuel cell

The principles explained below are based on [23] and will be briefly described. For a more details I recommend consulting this book.

The process that happens in the fuel cells (FC) is the recombination of hydrogen and oxygen to produce water and electric current.

$$2H_2 + O_2 \longrightarrow 2H_2O$$
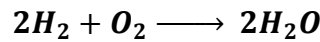
It can be seen that the hydrogen fuel is combusted in the reaction and a combination of electrical energy and, in a less quantity, heat energy is produced.

To understand how the reaction produces electric current, and where the electrons come from, the separate reactions, taking place at each electrode, must be considered.

At the anode of an acid electrolyte fuel cell, the hydrogen gas ionises, releasing electrons and creating H^+ ions (or protons).

$$2H_2 \longrightarrow 4H^+ + 4e^-$$
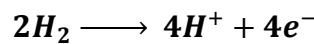
This reaction releases energy. At the cathode, oxygen reacts with electrons taken from the electrode, and H+ ions from the electrolyte, to form water.

$$O_2 + 4e^- + 4H^+ \longrightarrow 2H_2O$$

Obviously, for both these reactions to progress in a continuous way, electrons produced at the anode must pass through an electrical circuit to the cathode. Also, H^+ ions must pass through the electrolyte. An acid is a fluid with free H^+ ions which serves this purpose very well. Certain polymers can also be made to permit the movement of protons. These materials are called proton exchange membranes (PEM).

In all FCs the overall reaction is the same, but the reactions at each electrode are different. In an alkaline electrolyte FC, hydroxyl (OH^-) ions are available and mobile. At the anode, these react with hydrogen, releasing energy and electrons,

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and producing water. At the cathode, oxygen reacts with electrons taken from the electrode, and water in the electrolyte, forming new OH^- ions.

For the reactions occurring in each electrode to proceed continuously, the OH^- ions must be able to pass through the electrolyte instead of H^+ in PEM, and there must be an electrical circuit for the electrons to go from the anode to the cathode as in PEM.

There are limitations in current because the release of energy doesn't mean that the reaction proceeds at an unlimited rate. The reaction needs a minimal 'activation energy' to be realised as can be observed in Figure 3.4.
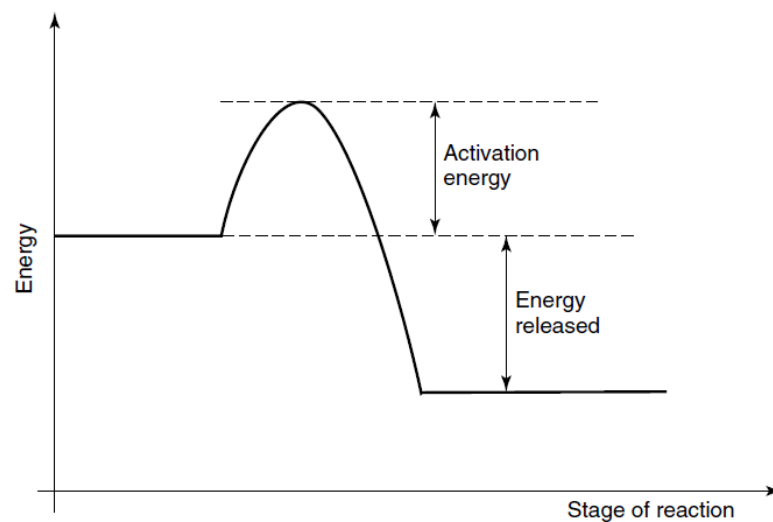
Figure 3.4: Classical energy diagram for a simple exothermic chemical reaction.

The three principal ways of dealing with the slow reaction rates are the followings:

- to use catalysts such as platinum,
- to raise the temperature.

There are many different types of fuel cell with different electrolytes and each electrode has different reactions in each case. The Table 3.1 presents different types of FC, some of their applications, the operating temperature and the mobile ion in the electrolyte.

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Table 3.1: Comparison of some types of fuel cell.

Fuel cell type	Mobile ion	Operating temperature	Applications and notes
Alkaline (AFC)	OH^-	50–200◦C	Used in space vehicles, e.g. Apollo, Shuttle.
Proton Exchange Membrane (PEMFC)	H^+	30–100◦C	Vehicles and mobile applications, and for lower power CHP systems
Direct Methanol (DMFC)	H^+	20–90◦C	Suitable for portable electronic systems of low power, running for long times
Phosphoric Acid (PAFC)	H^+	~220◦C	Large numbers of 200-kW CHP systems in use.
Molten Carbonate (MCFC)	CO_3^{2-}	~650◦C	Suitable for medium- to large-scale CHP systems, up to MW capacity
Solid oxide (SOFC)	$O2^-$	500–1000◦C	Suitable for all sizes of CHP systems, 2kW to multi-MW.

The fuel cell used in this study will be the AFC, the PEMFC or the DMFC fuel cell type. Indeed, the operating temperature for the considered application (the building sector) is 70°C.

It is noteworthy to mention that this work will serve not only to study the flexibility of using hydrogen as an energy vector on buildings, but also to give some basic results to the electrochemical laboratory of the University of Liège concerning the supposed demand that a building would ask to a system where a FC is presented.

The laboratory has a Proton Exchange Membrane Fuel Cell, the NEDSTACK 5kW PEM. Because the study they are going to do is confidential, all the data referring to the PEMFC that permitted to do the model was obtained in [24]. It is important to note that the inlet pressure in the PEMFC selected must be between 1 and 2 bar. So, the hydrogen storage that is done at high pressure must be expand with an expander system.

3.2.2. Electrolyser

The theory of electrolyser was described by *Christophe Coutanceau et al.* [15].

The global reaction happening in a water electrolysis system consists in the decomposition of water molecules:

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$$2H_2O \longrightarrow 2H_2 + O_2$$
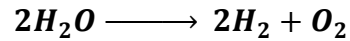
The water electrolysis system is composed of two electrodes (an anode where the oxidation takes place and a cathode where reduction of water occurs) and an electrolyte (ionic conductor). The reactions happening in the electrolyser are the reverse of the ones described in the fuel cell. The two electrodes are connected to an electric energy generator. The reaction can occur under different conditions: aqueous alkaline or aqueous acidic conditions at temperatures lower than 100°C, or using solid oxide electrolytes at temperatures higher than 700°C. Depending on the electrolytes used and the electrolysis cell temperature, water electrolysis cells are classified in three main categories:

- Alkaline electrolysis cell (AEC): the cell works at a temperature around 80°C, ionic species are hydroxyl ions (OH⁻), aqueous KOH or NaOH as electrolytic media;
- Proton exchange membrane electrolysis cell (PEMEC): the cell works at a temperature around 80°C, ionic species are hydronium ions (H⁺), perfluorosulfonic acid (PFSA) membranes as solid electrolytes;
- Solid oxides electrolysis cell (SOEC): the cell works at a temperature around 700°C, ionic species are oxide ions (O^{2-}), yttrium-stabilized zirconia as solid electrolytes.

Each electrolysis cell presents different reactions at both electrodes according to the ionic species transported through the electrolyte. Independently on the electrolytic media, the standard anode potential for the anodic reaction of water oxidation is:

$$E^0_{(O_2/H_2O)} = 1.23 \; V$$

while the standard cathode potential for all cathodic reactions of water reduction is:

$$E^0_{(H_2O/H_2)} = 0 \; V$$

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The standard cell voltage for the global reaction of water dissociation is 1.23 V independently on the electrolysis system. This value is only theoretic. The real voltage needed is higher because of the kinetic and diffusion losses also including the Joule effect. For the reaction to initiate an activation energy is needed as well as in the FC (Figure 3.4). The figure 3.5 represents the three systems previously explained.
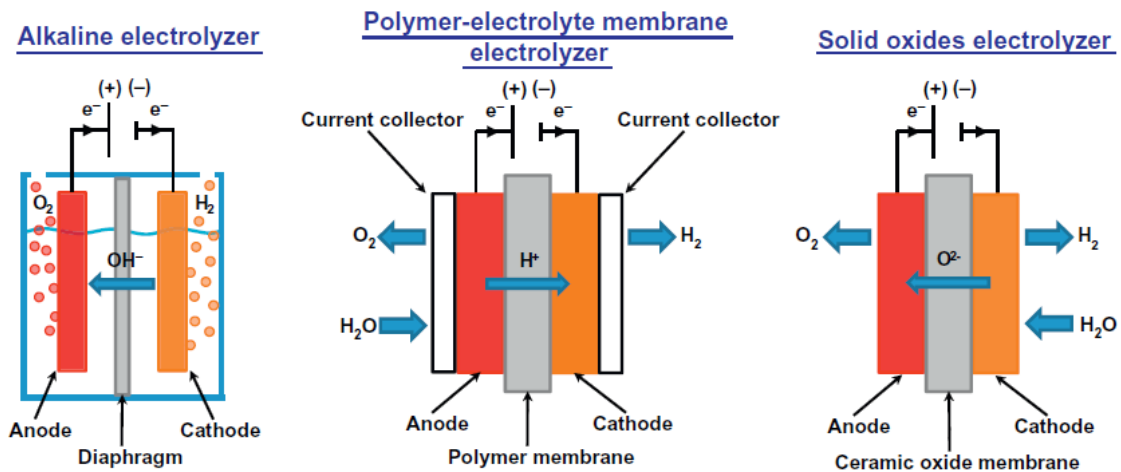
Figure 3.5: Working principle of the different water electrolysis cell systems.

The principal advantages and disadvantages of each electrolysis cell system are summarized in table 3.2.

It can be observed in Table 3.1, that depending on the conditions required for the electrolyser one or another technology will be used. The project focuses on the utility of hydrogen on residential buildings. Therefore, low range of power will be needed. Between the Alkaline or PEM, the last one has been chosen because recent studies have proven that high pressures can be achieved with this technology (range of 70 to even more than 100 bar) [27,28]. Furthermore, the Fuel Cell that was selected it was a PEMFC.

To achieve the high pressure in the electrolyser, a water pump is needed. The water pump requires less energy than a hydrogen compressor. Thanks to the possibility to work with electrolysers at high pressure, the work of hydrogen compressor, if it exists in the system, will be low.

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Table 3.2: Main advantages and disadvantages of Electrolysis Cell Systems [25,26].

	Alkaline Electrolysis	PEM Electrolysis	Solid Oxide Electrolysis
Advantages	Commercial technology. Non-noble catalysts. Long-term stability. Relatively low cost. MW range stacks. Cost effective.	Near-term technology. High current densities. High voltage efficiency. Good partial load range. Rapid system response. Compact system design. High gas purity. Dynamic operation.	Efficiency up to 100%. Thermoneutral voltage. Non-noble catalysts. High-pressure operation.
Disadvantages	Low current densities. Crossover of gases (degree of purity). Low partial load range. Low dynamics. Low operational pressures. Corrosive liquid electrolyte.	High cost of components. Acidic corrosive medium. Possibly low durability. Stacks below MW range.	Mediate-term technology. Bulky system design. Durability (brittle ceramics) no dependable cost information.

3.2.3. Batteries

The system of the project will be a hybrid system of electrical energy production. The electric power demanded by the system will be delivered by the battery when the PV panels doesn't deliver enough power and the fuel cell will serve to

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charge the battery when it attends a certain level of charge. For this reason, it is necessary to understand how a battery works and to have a global view of the different batteries available on the market.

Batteries can be defined as electrochemical generators recovering chemical energy as electrical work. They are constituted by two electrodes where the chemical reactions occur (being the electron conductors) and an electrolyte that is a pure ionic conductor but an insulator for the electrons. The batteries can be represented by the following general chemical equation:

$$a\ OX_1 + b\ RED_1 \longrightarrow c\ RED_2 + d\ OX_2$$
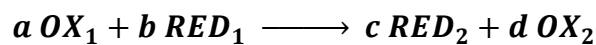
That means that in one of the electrodes (the cathode) a chemical reduction is done and in the other (the anode) a chemical oxidation happens.

The batteries can be divided in two main groups:

- Primary generators which are not rechargeable.
- Secondary generators which are rechargeable.

The primary generators are mainly characterized by:

- Non inversible reaction, therefore the general chemical equation only happens in one direction. The battery is charged at the beginning and then it is used for one discharge.
- Poor cyclability meaning that they have a bad yield. The charge and discharge cycle could not be interesting because of the big losses of the cell. Some of the cell are also not symmetric, meaning that the voltage that it is given by the batteries in discharge mode is lower than the one that it must be imposed in charge mode.
- Material degradation supporting mechanical stress due to dilatation, compression and other factors in the material than weakens it.

Some primary generators are exposed with their principal characteristics in the table 3.3.

Table 3.3: Different primary generators with their principal characteristics.

Type of cell	Leclanché (salt cell or 'dry cell')	Alkaline	Lithium
Δε (V)	1.5	1.5	1.5 to 3.7
Energy density (Wh/kg)	~ 30 – 50	80 – 160	250 – 300 (Li/MnO₂)
Lifetime (h)	20 – 30	50 – 60	> 5 years

The secondary generators are mainly characterized by:

- Acceptable cycling yield.

- Acceptable material degradation.

- Inversible reaction therefore the general chemical equation can happen in both directions. The charge and discharge mode can be cycled over the lifetime of the battery with littles degradation (depending in how the charge and discharge are done). Charge and discharge mode are represented in the Figures 3.6.a and 3.6.b.
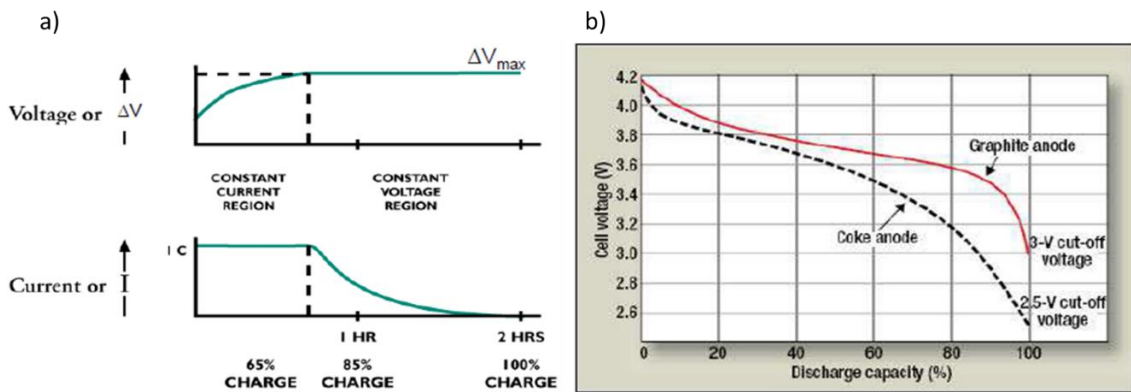
Figures 3.6: Representation of charge (a) and discharge (b) mode of a battery.

On the left figure the charging curve can be observed. It can be separated in two parts, the first one happens with an application of a continuous current until ΔV reach approximately ΔV_{max}. The second part is obtained when a continuous voltage is applied while the current decreases as the battery is getting charged until it reaches approximately I = 0. On the right figure, the discharging curve is illustrated. It is represented with two different materials for the anode. The

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performances depend on the followings criteria: admissible discharge depth (minimum voltage that can be achieved before damaging the system); intensity of the discharge current (if the discharge happens at high current the lifetime decrease); and the cut-off voltage (V at the end of discharge).

The discharge can be done at constant current, at constant power or at constant resistance. One remark, a longer flat will appear when the power of discharge is constant (it can be observed in the Figure 3.6.b when graphite anode is used).

Some secondary generators are exposed with their principal characteristics in the table 3.4.

Table 3.4: Comparison between some common batteries.

Batteries	Lead	Ni-Cd	Ni-MH	Ni-Zn	Li-ion
Δε (V) per cell	2.1	1.2	1.2	1.65	3.7
Energy density (Wh/kg)	20 – 40	40 – 60	30 – 80	~100	100 – 265
Charge-discharge yield	50 %	70 – 90 %	66 %	---	99.9 %
Auto-discharge	5 %/months	10 – 20 %/month	20 %/month	30 %/mois	5 – 10 %/month
Lifetime years	4 – 5	2 – 3	2 – 4		2 – 3
Number of charge cycles	500 – 1200	2000	500 – 1000	400 – 1000	1200
Disadvantages	Presence of lead and acid (recyclable, but pollutant). Weak energy density. Low charge-discharge yield.	Quick auto-discharge. Sensitive to memory effect. Environmental issues.	Lifetime lower than Ni-Cd. Metal hybrids are difficult to recycle.	Degradation of Zn. Quick auto-discharge.	Degradation of the materials, even without use. Low discharge depth: 10–20%. Low charge-discharge currents. Li dendrite growth -> short-circuits.

As can be observed in the Table 3.4, if a comparison of the batteries is done, the logical selection for this work would be a Li-ion battery. Furthermore, this kind of battery doesn't have memory effect and is the most frequently used battery in the market nowadays.

All the information presented in this section was obtained from [29].

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3.3. Mechanical part of the system

The mechanical part of the system developed for the project was composed of a water pump, an expander system located before the hydrogen tank and depending on the necessity of the system to reduce the volume of hydrogen stored, the system will contain a hydrogen compressor.

In the following subsections these mechanical parts will be explained in more details.

3.3.1. Water pump

Water pumps are usually used in hydrogen production systems to provide the amount of water required by the electrolyser. However, recent experiments have proven that it is possible to develop electrolysers able to work at high pressure [27]. Consequently, water at high pressure will be needed. Therefore, additional work must be performed for the development of performant water pumps for the increasement of water pressure before entering the electrolyser.

In this work one model of a water pump will be designed, doing several hypotheses, because no water pump with the required characteristics was found on the market.

3.3.2. Expander

Hydrogen expanders are usually used industrially for hydrogen cryogenic storage. The transformation of hydrogen from gas to liquid state requires to drop the temperature up to 22 K. Thanks to hydrogen expander/turbines the enthalpy drops causing a significant cool down of hydrogen temperature.

Almost all gases cool down at room temperature during an "adiabatic expansion" through a valve. However, Helium, Neon and Hydrogen heat up, phenomena named Joule-Thomson effect. Thanks to this property of Hydrogen, an expander

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system can be done in various ways. The followings details explain two options of expansion:

- In laboratories and another sites Hydrogen is usually stored before use. The stored hydrogen is also compressed. Consequently, there exists a compression work that has been made. Normally, some laboratories also receive the hydrogen tanks full of hydrogen and when the vessels are empty they replace them. Subsequently, they are not concerned into the energy recovery of hydrogen so, they use a hydrogen regulator (valve) to lower pressure before use it in a fuel cell, for example.

- Another option is proposed in this project. It consists in hydrogen expanding to a level of pressure at which the associated temperature is lower than the minimal temperature required for the normal operation of the fuel cells. Then, a valve does the other stage of pressure at which hydrogen will reach the desired pressure before entering in the FC. Due to the hydrogen properties it will warm up to the minimal operational temperature.

Nowadays, it is particularly difficult to find the expander system required for the project. Consequently, a recovery system is also modelled.

3.3.3. Hydrogen compressor

The information obtained and presented in this subsection were collected from [30].

Hydrogen compression is realized by a machine that increases the pressure of the gas by reducing its volume. However, the low molecular weight of hydrogen requires the use of a volumetric compressor instead of a centrifugal one, in order to gain efficiency. Furthermore, like any compressed gas, the energy used for hydrogen compression not only increases its pressure but also the temperature. Hydrogen compressors can be categorised in mechanical and non-mechanical.

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The main difference between these compressors is the lack of moving parts in the second ones. Their principal characteristics are presented below:

- **Mechanical compressors:** two principal mechanical compressors are used in the market, the *piston compressor* and the *piston-metal diaphragm hydrogen compressor* which are represented in Figures 3.7.a and 3.7.b respectively. The first one is defined by one or two stage units of an electro-hydraulically driven system that is non-lubricated. The liquid is refrigerated, the compressor includes an electric motor, a hydraulic oil tank, high pressure gas intensifier and intensifier shifting mechanism. In the second one, the gas is isolated from the piston and the other components by a set of metal diaphragms.
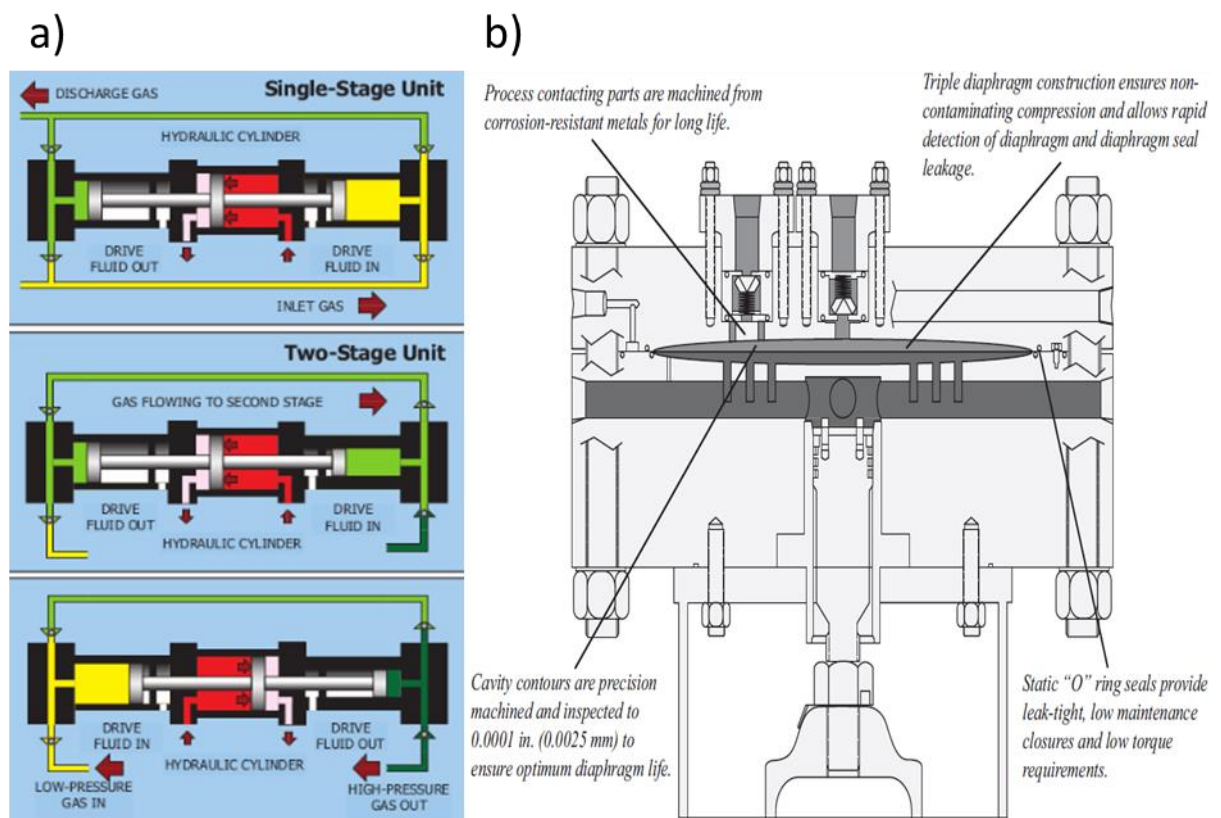
Figure 3.7: a) On the left figure, a schematic diagram of one and two stage compression unit [31]. **b)** On the right figure, a diagram of a metal diaphragm hydrogen compressor is presented [32].

- **Non-mechanical compressors:** two principals non-mechanical compressors represent this category, the *electrochemical hydrogen compressor* and *metal hydride hydrogen compressors (MHHC)*. The operating principle of

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both compressors are represented respectively in Figures 3.8 and 3.9. The first one is used instead of mechanical compressor for low flow rate of hydrogen driven to high pressure because is more efficient [33]. It has similar principle of working as electrochemical cells, two electrodes (anode and cathode) and a membrane electrode assembly. When a difference of potential is applied, the hydrogen that enters at a pressure of P_1 is oxidised to H^+. These ions pass through the membrane, then they are reduced to H_2 at a pressure $P_2 > P_1$, if the cathode compartment is hermetic. Whereas hydrogen and power are provided, the hydrogen compression is maintained by the electrochemical reaction. The MHHC behaviour can be compared to a thermal engine because of the performance of reversible metal hydride alloys to compress hydrogen. The working principle of MHHC is based on heat and mass transfer during absorption and desorption process of hydrogen [34]. A single-stage of the compressor is composed by a compartment filled with a reversible metal hydride alloy. Four processes (represented in the figure 3.9) can describe the functionality of the compressor [34]:

- A-B: Hydrogen is absorbed into the alloy sheet at low temperature (T_c) and at low pressure (P_s).
- B-C: The compartment is heated from T_c to T_h with compression taking place at the same time.
- C-D: Compressed hydrogen is desorbed and released at high temperature and high pressure (P_d).
- D-A: The compartment is cooled down until reach the value of T_c is reached.

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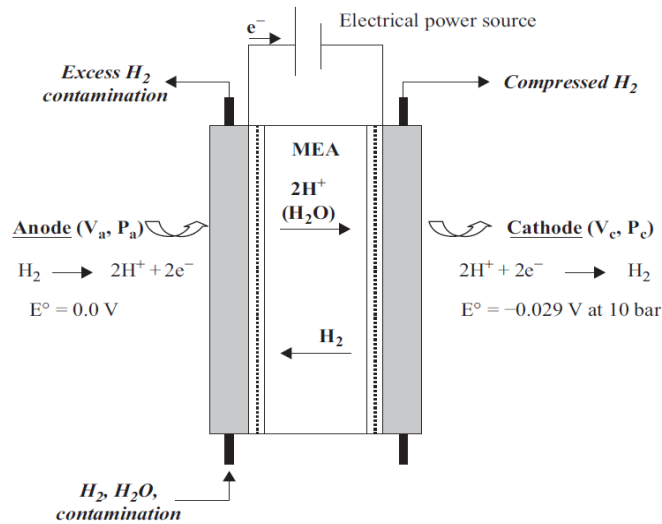
Figure 3.8: Working principle of the electrochemical hydrogen compressor [35].
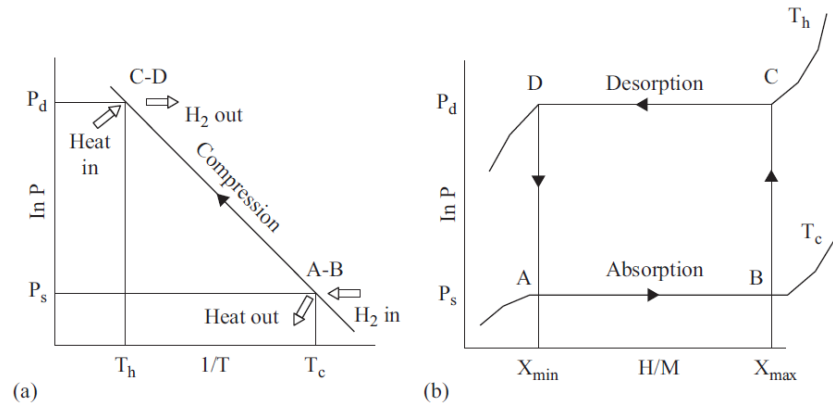
Figure 3.9: Working principle of a single stage metal hydride hydrogen compressor [36].

3.4. Hydrogen storage

Hydrogen storage is principally related to cases with low-power applications, which would not justify the cost of fuel-processing equipment. It is also a way of storing electrical energy from renewable sources such as solar panels, wind turbines and hydroelectric power, whose production sometimes must be suspended even if they can still be producing. Electrolysers might be used to convert the electrical energy to hydrogen during these periods of time.

The principal problem with hydrogen, even if it has one of the highest specific energies (120000 kJ/kg), is its very low density (0.084 kg/m^3 at Standard Conditions 1 bar and 288.15 K) and its low energy density (10080 kJ/m^3).

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Consequently, a very high pressure is needed if a considerable mass of hydrogen has to be stored in a small space. To arrive at liquid form hydrogen must be compressed and cooled down at about 22 K and even in liquid form its density is quite low, around 71 kg/m^3.

There are various methods for hydrogen storing:

- Compression in gas tanks;
- Storage as a cryogenic liquid;
- Storage in a metal absorber.

The most widely used method and the one used in this project is the storage of hydrogen in gas tanks. Hydrogen is stored in this way in a widely amount of industrial and researching establishments, and in the most local companies that work with this technology can supply cylinders of various dimensions.

A comparative data for two types of cylinders will be given in Table 3.5.

Table 3.5: Comparative data for two cylinders used to store hydrogen at high pressure. The first one is a conventional steel cylinder and the second one a composite tank (more expensive about 3 times the cost of conventional steel cylinders of the same capacity).

	2 L steel, 200 bar	147 L composite, 300 bar
Mass of empty cylinder (kg)	3.0	100
Mass of hydrogen stored (kg)	0.036	3.1
Specific energy (kWh/kg)	0.47	1.2
Volume of tank (approx.)	2.2 L (0.0022m^3)	220 L (0.22m^3)
Mass of H$_2$ per litre	0.016	0.014

The principal advantages of storing hydrogen as compressed gas are the following:

- Simplicity
- Indefinite storage time
- No hydrogen purity limits.

This method of hydrogen storing is widely used in locations where the demand of hydrogen is not constant and not so high.

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3.5. Safety of hydrogen storage

Hydrogen is the gas with the lowest molecular weight. It has the highest thermal conductivity, molecular velocity, and the lowest density and viscosity of all gases. Hydrogen has a leak rate through small orifices faster than all other gases. Hydrogen escapes 2.8 times faster than methane and 3.3 times faster than air. Furthermore, hydrogen is a highly volatile and flammable gas, and hydrogen-air mixtures can explode.

Hydrogen needs to be handled by professional people. Systems need to be monitored for such leaks regularly and designed carefully.

However, it should also be mentioned, that hydrogen is not more dangerous, and in some features, it is even safer than other fuels usually used. A comparison of security aspects for hydrogen and two others gaseous fuels is done in Table 3.6.

Table 3.6: Properties relevant to safety for hydrogen and two others commonly used gaseous fuels.

	Hydrogen	Methane	Propane
Density, kgm−3 at NTP	0.084	0.65	2.01
Ignition limits in air, volume% at NTP	4.0 to 77	4.4 to 16.5	1.7 to 10.9
Ignition temperature, ◦C	585	540	487
Min. ignition energy in air, MJ	0.02	0.3	0.26
Max. combustion rate in air, ms−1	3.46	0.43	0.47
Detonation limits in air, volume%	18 to 59	6.3 to 14	1.1 to 1.3
Stoichiometric ratio in air	29.5	9.5	4.0

As shown in Table 3.6, the biggest issue of hydrogen is its minimum ignition energy, indicating that a fire could be initialised very easily. In fact, the energies shown here are very low. The smallest spark could ignite each of these fuels. However, the minimal concentration of hydrogen needed for detonation is much higher (18% by volume of air) than for the other gases (6.3% for Methane and 1.1% for Propane) and liquid fuels such as diesel (0.6%) and gasoline (1.4%). The concentration limit for ignition is similar to the one of methane in the lower aspect but it is considerable lower comparing to propane. An advantage of

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hydrogen is the ignition temperature which is higher comparing to the other two fuels.

The range of concentrations needed to cause detonation must be carefully controlled to prevent the accumulation of hydrogen in confined places. Fortunately, the high diffusion factor of hydrogen (shown in Table 1.1), guarantees that hydrogen is the fastest dispersing gas.

Another safety problem that can occur with hydrogen is that when it burns, the flame is invisible to human eyes, so special cameras must be used to ensure the safety installation. Nevertheless, taking all parameters into account, the danger that can present hydrogen is not bigger than any other flammable liquids or gases that are currently used. In fact, the dangers are different. The hydrogen is usually employed by professional people every day but, always with strictly rules of security.

The metal for hydrogen the pressure tanks has to be selected very carefully because hydrogen is a very small molecule and because of its high diffusion it passes through some materials that are impermeable to other gases. This is the reason why the hydrogen pipelines are coated with special polymers.

Some safety precautions must be considered for leaks when high pressure is present, to avoid a cylinder act as a torpedo and produce considerable damage. Nevertheless, this method is widely and safely used. For example, in vehicles where the pressure of the tanks achieves 700 bar (Toyota Mirai). For instance, the tanks pressurised has liberation valves, which will safely vent gas in the event of a fire. Some regulators are attached to the tanks to prevent the hydrogen's ignition.

The information from the section 3.4 and 3.5 is based on [23] and [7].

4. Modelling of the components hydrogen-based energy storage system

4.1. Photovoltaic panels

The model of the photovoltaic (PV) panels is composed of an irradiance model and an equation defining the efficiency of the PV panel. The PV panels efficiency depends on the ambient temperature (T_a), and the irradiance that reaches the PV panels. The model is represented in figure 4.1.

The inputs of the model are the direct horizontal irradiation S_h, the global horizontal irradiation G_h and T_a. The parameters are the longitude L, the latitude ϕ, the declination angle of the panel i, the azimuth angle γ, the albedo ground a*, and the characteristics of the panel are given in the **ANNEXE**. The outputs are the power by m^2 at each time and the energy production.
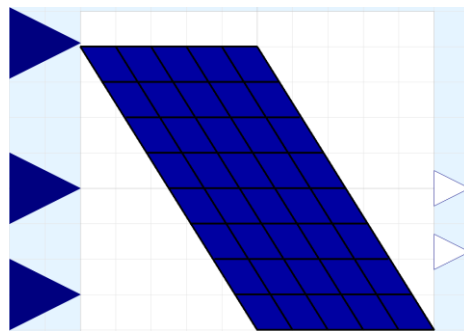
Figure 4.1: Representation of the PV model with inputs and outputs.

The irradiation model can be defined as follows: first, the hour angle ω is determinate. The hour angle converts the true solar time (TST) into the number of degrees the sun moves across the sky. The hour angle is 0° at solar noon. Since the Earth rotates 15° per hour, each hour away from solar noon corresponds to an angular motion of the sun in the sky of 15° [37].

Brussels is located at 50.85° N latitude and 4.35° E longitude. The panels are supposed to have an i = 20° and γ = 0.

The standard time (2 PM) is the time indicated by public clocks and it is obtained by the following equation:

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$$ST = MST + \frac{L}{15} + C_1 + C_2 \qquad \text{Equation PV1}$$

with MST the mean solar time, L the longitude and $C_1 = 1$, $C_2 = 0$ in winter and $C_2 = 1$ in summer.

The true solar time, TST, is given by:

$$TST = MST + \frac{ET}{60} \qquad \text{Equation PV2}$$

The difference between the TST and the MST is represented by the equation of time ET as:

$$ET = -0.00002 + 0.4197 \cos(\beta) - 7.3509 \sin(\beta) - 3.2265 \cos(2\beta) -$$
$$9.3912 \sin(2\beta) - 0.0903 \cos(3\beta) - 0.3361 \sin(3\beta) \qquad \text{Equation PV3}$$

where $\beta = \frac{360}{366} n$, while n is the number of days. 'n' is defined as $ceil\left(\frac{time}{24*3600}\right)$ this means that the variable *time* (time of simulation in seconds) is divided by 24h (in a day) and 3600 seconds (in one hour).

Finally, the hour angle is given by:

$$\omega = (TST - 12) \cdot 15 \qquad \text{Equation PV4}$$

Knowing the declination δ, the latitude φ and the hour angle ω, the solar altitude h and the azimuth angle a at the location, date and time desired can be determined with:

$$\begin{aligned} \cos(h)\sin(a) &= \cos(\delta)\sin(\omega) \\ \cos(h)\cos(a) &= \cos(\delta)\cos(\omega)\sin(\phi) - \sin(\delta)\cos(\phi) \quad \text{Equation PV5} \\ \sin(h) &= \cos(\delta)\cos(\omega)\cos(\phi) + \sin(\delta)\sin(\phi) \end{aligned}$$

There are some cases such as, the quantities related to sunrise and sunset (h = 0) that are denoted by the index "0" while those related to solar noon (12h t, a = ω = 0) with the index "n".

- Height at solar noon: $h_n = \arcsin(cos(\delta - \phi))$
- Hourly angle at sunset: $\omega_0 = \arccos(-tan(\phi) \cdot tan(\delta))$

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- Azimuth at sunset:
$$a_0 = \arccos\left(-\frac{sin(\delta)}{cos(\phi)}\right)$$

- Duration of the day (in hours):
$$DayDur = 2 \cdot \frac{\omega_0}{15}$$

-
$$TST_0 = \frac{\omega_0}{15} + 12$$

-
$$ST_0 = TST_0 - \frac{ET}{60} + \frac{L}{15} + C_1 + C_2$$

Once all these parameters are calculated and the S_h and G_h are given, the global irradiation reaching the sloping surface $G_{i,\gamma}$ can be obtained. To achieve the result of this irradiance the followings equations must be resolved.

First, the direct irradiation that reaches the declined surface is calculated as:

$$S_{i,\gamma} = I \cdot (\sin i \cdot \cos h \cdot \cos(a - \gamma) + \cos i \cdot \sin h) \qquad \text{Equation PV6}$$

Then, the diffuse solar irradiation reaching the tilted surface can be estimated as:

$$D_{i,\gamma} = D_h \cdot \frac{1 + \cos i}{2} + a^* \cdot G_h \cdot \frac{1 - \cos i}{2} \qquad \text{Equation PV7}$$

with $G_h = S_h + D_h$; and a^* is the albedo ground that in this project is assumed as 0.2.

Finally, the $G_{i,\gamma}$ can be calculated as:

$$G_{i,\gamma} = S_{i,\gamma} + D_{i,\gamma} \qquad \text{Equation PV8}$$

When the global irradiation that reaches the surface of the panels is obtained, the electrical power produced is the interesting parameter the system need from the model of the PV panels. For that, the efficiency of the PV panels will be necessary. The definition of the efficiency can be defined as:

$$\eta_{PV} = \eta_{ref} \cdot \left(1 - \beta_{ref} \cdot \left(T_a - T_{ref} + (T_{NOCT} - T_a) \cdot \frac{G_{i,\gamma}}{I_{NOCT}}\right)\right) \qquad \text{Equation PV9}$$

with η_{ref} as the reference efficiency of the PV panels (variable that can be obtained from the characteristics of the PV panels) in this case is 0.158; β_{ref} as the temperature coefficient for the crystalline silicon modules that depends on the material properties, in this case is 0.004 [17]; T_{ref} is the reference temperature of 25 ºC; T_{NOCT} is the Nominal Operating Cell Temperature given by the constructor and it's 46 ºC; and I_{NOCT} is the irradiance at NOCT that is equal to 800 W/m^2. So, as can be observed, the efficiency of the PV panels will change because the ambiance temperature and the irradiance reaching the PV panel change.

To finalize the model of the PV panels, the electrical power production can be defined as:

$$\dot{W}_{elec} = \eta_{PV} \cdot G_{i,\gamma}$$
<div align="right">Equation PV10</div>

4.2. Electrolyser

The electrolyser can be constructed as a black box where inputs, parameters and outputs are considered. The inputs of the electrolyser are the electrical power that it is not consumed by the building and the one that it is not used to charge the electrical battery. The parameters are the number of cells, the inlet temperature and the operating pressure. The outputs are the water mass flow rate needed to do the electrolysis, the hydrogen mass flow rate produced, and the mass of hydrogen produced. As the oxygen valorisation it is not considered in this work this output it is not considered. The representation of this black box is illustrated in Figure 4.2.
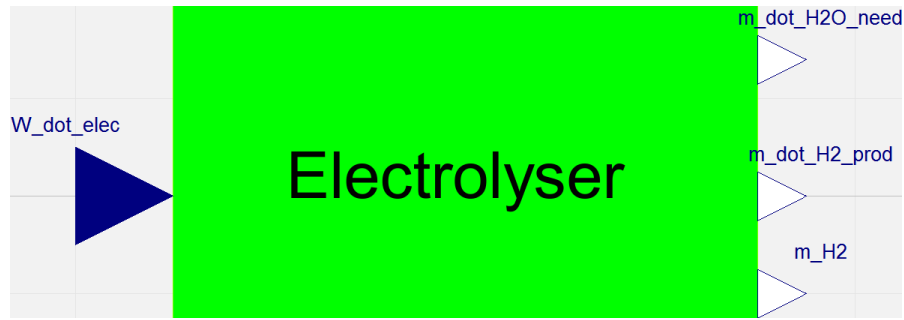
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Figure 4.2: Representation of the diagram of the electrolyser with inputs and outputs.

The electrolyser was modelled from the experimental polarisation curve represented in Figure 4.3 [27].
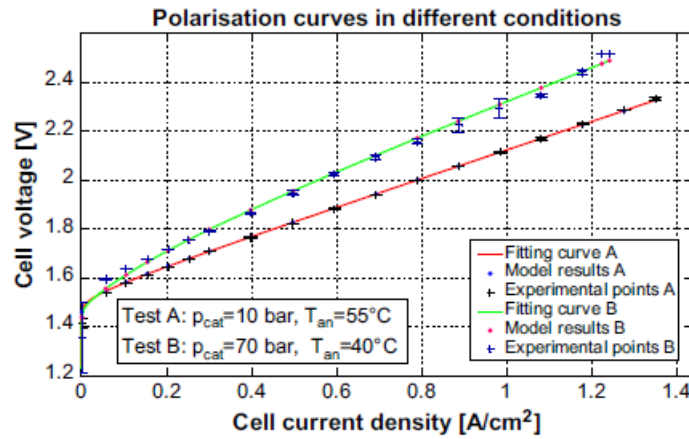
Figure 4.3: Polarisation curve in different conditions of pressure and temperature.

The following equation express the experimental equation obtained from the Figure 4.3 at 70 bar.

$$V_{TP_{cell}} = \begin{cases} 0.7551 * I_{cm^2} + 1.572 & I_{cm^2} > 0.05 \\ e_{rev_{TP}} & I_{cm^2} < 0.05 \end{cases} \qquad \text{Equation Elect1}$$

Where V_{TPcell} is the cell voltage needed for the chemical electrolyse at 70 bar and the temperature of the Test B, I_{cm2} is the cell current density in the same conditions and e_{revTP} is the reverse voltage at the temperature T and pressure P defined in the following equation:

$$e_{rev_{TP}} = e_{rev_0} + \frac{R*T}{2*F} * \ln\left(\frac{P}{P_0}\right) \qquad \text{Equation Elect2}$$

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Where e_{rev0} = 1.476 V and is the reference voltage at the reference temperature T_0=293 K and pressure P_0 = 1 bar, R = 8.314472 [J/(K·mol)] is the constant of ideal gases and F = 96485 C is the Faraday constant.

The size of the cell was defined to ensure that the cell works most of the time between 0.2 and 0.6 A/cm². So, the size of the cell is 60 cm². $I_{cell} = size * I_{cm^2}$

Using the equation the Equation Elect1 and the energy that must be stored with the following correlations, we define the quantity of hydrogen produced and its volume.

It is well-known that the electrical power is defined as:

$$\dot{W}_{elec} = n_{tot} * V_{TP_{cell}} * I_{cell} \qquad \text{Equation Elect3}$$

where n_{tot} = 20 is the total number of cells in the electrolyser.

Under nominal operating conditions at room temperature (20 ºC), and 1 atm pressure, the ideal potential V_i is 1.233 V. The V_i is useful for electrolysis and is used for hydrogen production [38]. But considering that the electrolyser doesn't work under nominal condition, the Equation Elect4 [39] is considered.

$$V_i = \frac{\Delta G}{2*F} \qquad \text{Equation Elect4}$$

where $\Delta G = 285.840 - 163.2 * T$ is the Gibbs free energy change (J/mol) of hydrogen gas for a given temperature T (K) [39]. It can be associated with the following expressions, which are based on electro-chemistry. To know the mass and the volume of hydrogen produced first, the mass flow rate of hydrogen produced at P = 70 bar must be known:

$$\dot{m}_{H2} = \frac{MM_{H2}*n*I_{cell}}{2*F} \text{ [kg/s]} \qquad \text{Equation Elect8}$$

where ρ_{H2} is the density [kg/m³] of hydrogen at T and P of the Test B on Figure 4.3. The mass of hydrogen produced is defined as:

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$$m_{H2} = \int_0^t \dot{m}_{H2} \cdot dt \qquad \text{Equation Elect9}$$

And the volume as:

$$V_{H2} = \frac{m_{H2}}{\rho_{H2}} \qquad \text{Equation Elect10}$$

Then, as logical for an installation of the system, the hydrogen is produced in an electrolyser using water. Considering the chemical equation of the production of H_2 it can be observed that 2 mols of water produce 2 mols of H_2, so:

$$2H_2O \longrightarrow 2H_2 + O_2$$
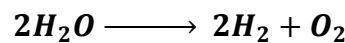
Knowing that the molar mass of each element is:

$$MM_O = 16\frac{g}{mol} \quad ; \quad MM_H = 1\frac{g}{mol}$$

The mass of water produced can be calculated:

$$m_{H_2O} = m_{H_2} * \frac{n_{H_2O}*MM_{H_2O}}{n_{H_2}*MM_{H_2}} = m_{H_2} * \frac{2*(2*MM_H+MM_O)}{2*(2*MM_H)} \quad \text{Equation Elect11}$$

The electrochemical hydrogen energy per second (useful power) which corresponds to the ideal Hydrogen produced can be defined as:

$$\dot{W}_{H_2} = n_{tot} * I_{cell} * V_i \qquad \text{Equation Elect12}$$

Finally, the efficiency of the electrolyser can be defined as the ratio between the mass of hydrogen produced and the mass of hydrogen that would be produced theoretically by the inlet energy:

$$\eta_e = \frac{m_{H_2 real}}{m_{H_2 theoretic}} = \frac{m_{H_2 real}}{\frac{Energy}{PCI}} \qquad \text{Equation Elect13}$$

4.3.   Fuel cell

The fuel cell can be reflected as a black box (Figure 4.4) where inputs, parameters and outputs are considered. As inputs the fuel cell has the hydrogen mass flow rate required to produce the electrical power needed by the battery to charge. As parameters, the number of cells and the stoichiometry factor of O_2 and H_2. And as outputs, the air mass flow rate needed to realize the chemical reaction, the mass of hydrogen used, the electrical power produced at each time and the heat power produced that can be valorised to heat water for a domestic hot water installation.
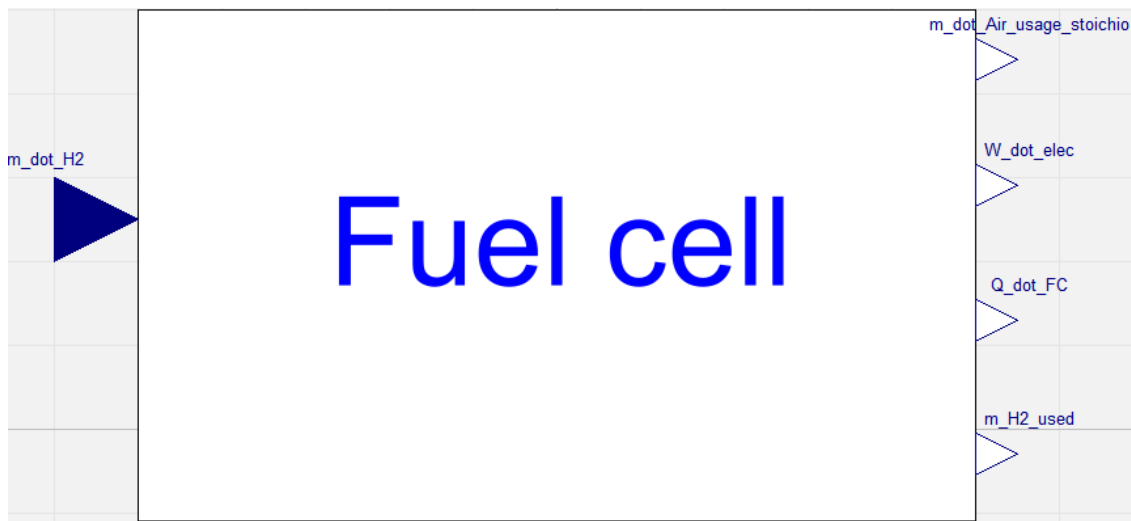
Figure 4.4: Representation of the diagram of the electrolyser with inputs and outputs.

The Fuel Cell is modelled using the polarization curve for 5 kW PEM Fuel Cell power stack (NEDSTACK FCS) [24] because the same FC is going to be used in the electrochemical laboratory of the University of Liège. In this way, the laboratory could use the data obtained by this model to have a first theoretical approximation of the performances of the FC connected to a system integrated in buildings.

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Figure 4.5: Polarisation curve of NEDSTACK FCS 5 kW.

The Figure 4.5 (FC_1) shows the power- current and the voltage-current characteristics of the stack. The current produced is proportional to the hydrogen and air flow rates consumed. The relationship between the power produced and the hydrogen and air consumed is described in the followings equations obtained from [23].
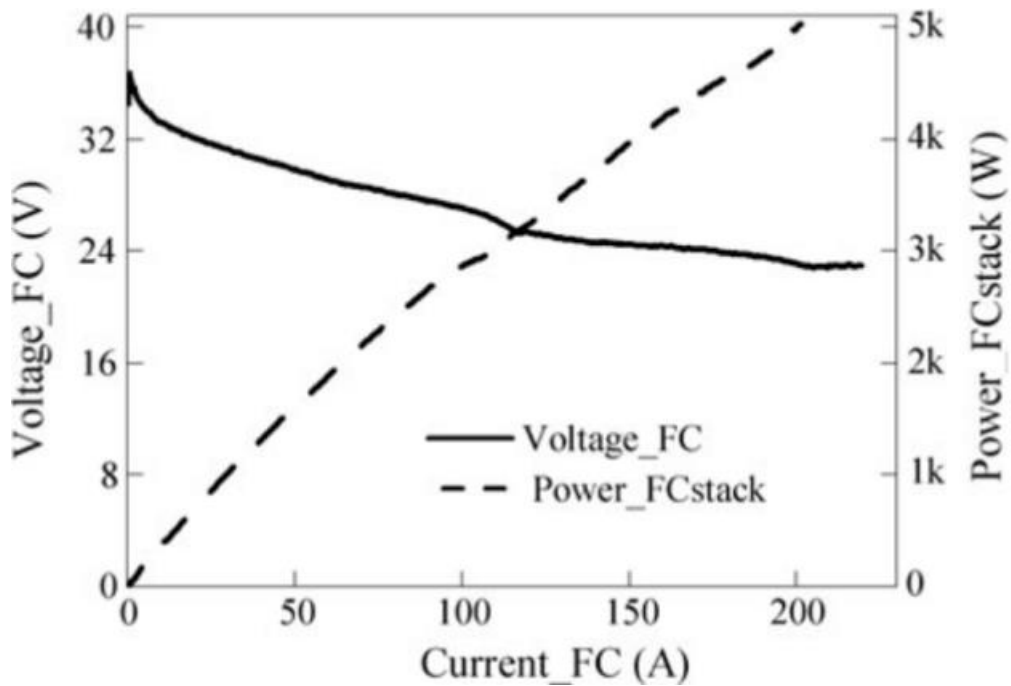
The simple FC reaction is:

$$2H_2 + O_2 \longrightarrow 2H_2O$$
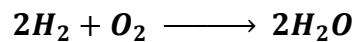
Two moles of hydrogen combined with one mole of oxygen will provide 2 moles of water (H_2O) and energy. This will produce exactly 4 F of charge; two electrons are transferred for each mole of hydrogen. Usually, the hydrogen and oxygen are both supplied in higher quantity than the stoichiometric rate to allow the electro-chemical reaction to occur.

This stoichiometry factor can be expressed as a variable, λ is normally used. For the FC used, the stoichiometry factors are 2 and 1.25 for oxygen and hydrogen respectively. Note also that the stack has 40 cells.

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Thanks to the Polarisation Curve of the Figure 4.5, the following relationships between current, voltage and electrical power can be made. Knowing that the electrical power is:

$$\dot{W}_{elec} = V_c \cdot I \cdot n \qquad \text{Equation FC1}$$

with V_c as the voltage of each cell in the stack, I the current produced and n the number of cells in the stack. So, $V = V_c \cdot n$ it is the total voltage produced in the stack. In the model the production of electrical power is the variable that orders the system of the FC to work. The equation of the current produced can be obtained from the polarisation curve (Figure 4.5):

$$I = \begin{cases} 0.02755 \cdot \dot{W}_{elec} & \dot{W}_{elec} < 450 \; [W] \\ 2 \cdot 10^{-6} \cdot \dot{W}_{elec}^2 + 0.0286 \cdot \dot{W}_{elec} - 0.9969 & \dot{W}_{elec} \geq 450 \; [W] \end{cases} \qquad \text{Equation FC2}$$

The total voltage produced is:

$$V = \begin{cases} -0.0005 \cdot I^3 + 0.0296 \cdot I^2 - 0.6049 \cdot I + 37 & I < 30 \; [A] \\ -2 \cdot 10^{-6} \cdot I^3 + 0.0008 \cdot I^2 - 0.1516 \cdot I + 35.332 & I \geq 30 \; [A] \end{cases} \qquad \text{Equation FC3}$$

The heat produced by the FC ($\dot{Q}_{FC}$) according to the electrical power produced will be:

$$\dot{Q}_{FC} = \dot{W}_{elec} \cdot \frac{1.25}{V_c - 1} \qquad \text{Equation FC4}$$

Once the power demanded is known and the current and voltage are obtained, the air and hydrogen needed to produce the electrical power can be estimated.

The generic chemical equation can be transformed in two equations, to express the oxygen and hydrogen contribution.

The chemical equation produced in the cathode is:

$$O_2 + 4H^+ + 4e^- \longrightarrow 2H_2O$$

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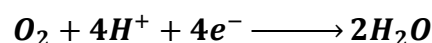
So, the Oxygen contribution can be analysed. From the basics of the electrochemical equations it is known that:

$$q = 4F \cdot m_{O_2}$$
<div align="right">Equation FC5</div>

with q as the charge, F the Faraday constant and m the mass of the component. If the last equation is divided by time, is rearranged and transformed not only for one cell but for the stack, it can be obtained:

$$\dot{m}_{O_2} = \frac{I \cdot n}{4 \cdot F} \left[\frac{moles}{s}\right]$$
<div align="right">Equation FC6</div>

with $\dot{m}_{O_2}$ is the total oxygen flow rate.

Combining the Equation FC1 with FC6 and transforming in kg/s is obtained:

$$\dot{m}_{O_2} = \frac{MM_{O_2} \cdot \dot{W}_{elec}}{4 \cdot F \cdot V_c}$$
<div align="right">Equation FC7</div>

with MM_{O_2} as the molar mass of O_2 in kg/mole that it is equal to $32 \cdot 10^{-3}$.

Usually, the oxygen used is derived from air, so the Equation FC7 must be adapted to air usage. The molar proportion of oxygen in air is 0.21, and the molar mass of air (MM_{Air}) is $28.97 \cdot 10^{-3}$ kg/mole. In practical mode the airflow is above stoichiometry to permit the cell to have enough oxygen for the reaction. This stoichiometry factor is given above. So, the new equation is:

$$\dot{m}_{Air} = \lambda_{O_2} \cdot \frac{MM_{air} \cdot \dot{W}_{elec}}{0.21 \cdot 4 \cdot F \cdot V_c}$$
<div align="right">Equation FC8</div>

The hydrogen flow rate is derived in a similar way to the production of oxygen, except that the chemical equation resulting in the anode is:

$$2H_2 \longrightarrow 4H^+ + 4e^-$$
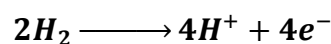
So, there are two electrons for each mole of hydrogen. As a result, the principle of the Equation FC6 change as:

$$\dot{m}_{H_2} = \frac{I \cdot n}{2 \cdot F} \left[\frac{moles}{s} \right]$$ Equation FC9

Combining the Equation FC1 with FC9 and transforming in kg/s gives:

$$\dot{m}_{H_2} = \frac{MM_{H_2} \cdot \dot{W}_{elec}}{2 \cdot F \cdot V_c}$$ Equation FC10

Using the stoichiometry factor for the hydrogen is obtained the final equation for the mass flow rate of hydrogen used in the FC to produce the power demanded.

$$\dot{m}_{H_2,stoichio} = \lambda_{H_2} \cdot \dot{m}_{H_2}$$ Equation FC11

The water production depends also on the demand of the electrical power. Therefore, water is produced at the rate of one mole for every two electrons, as it can be observed in the chemical equation produced in the cathode that it is delivered above.

$$\dot{m}_{H_2O} = \frac{MM_{H_2O} \cdot \dot{W}_{elec}}{2 \cdot F \cdot V_c}$$ Equation FC12

with MM_{H_2O} = 18.02·10^{-3} kg/mole that is the water molar mass.

Finally, it can be defined the cell efficiency, that it is:

$$\eta_{cell} = \frac{V_c}{E} \cdot 100$$ Equation FC13

with E as the theoretical maximum voltage that can be calculated as:

$$E = \frac{\Delta h}{2 \cdot F}$$ Equation FC14

with Δh as the Low Heating Value (LHV) of H$_2$ that it is equal to 241830 kJ/kmol. This equation gives the reversible open circuit voltage of the hydrogen FC.

4.4. Batteries

The batteries are modelled as a control volume that store electrical energy. The battery used in this project is POWERWALL 2AC of Tesla, a Li-ion battery. The characteristics of this battery are presented in the **ANNEXE**. Unfortunately, the characteristic curve of charging-discharging is not given in the datasheet. The model of the battery can be defined as a black box with the followings characteristics:

Figure 4.6: Battery model.

The inputs of the battery are the power received for charging, and the one demanded for the residential building (discharge power). As parameters, the battery has the internal voltage, the efficiency, the initial state of charge (SOC) and the capacity of the battery. Finally, the outputs are the SOC and the power demanded to the battery.

First, it was considered that the efficiency of the cycle charge-discharge of the battery affects only the charge. This hypothesis was made because it is not possible to know how much of this efficiency affects the charge and how much affect the discharge.

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$$\dot{W}_{elec,bat} = \dot{W}_{charge} * \eta_{bat} \qquad \text{Equation Bat1}$$

Knowing the power of charge and the demand of the residential building, the energy of the battery can be obtained doing the integration of the difference between both:

$$E = \int \left[\max(0, \dot{W}_{elec,bat}) + \min(0, \dot{W}_{discharge})\right] dt \qquad \text{Equation Bat2}$$

Finally, once the energy of the battery is obtained, the SOC can be calculated as:

$$SOC = \frac{E}{E_{maxi}} * 100 \qquad \text{Equation Bat3}$$

4.5. Water pump

The model of the pump considered not only drive water from the water tank to the electrolyser but also increase the pressure of water from low pressure to high pressure.

Some assumptions were done to do the model:

- The water pump is a volumetric pump.
- The isentropic efficiency used to do the model was consider a constant parameter that can be changed.
- The inlet pressure defined as parameter can change but it is not recommended.
- The outlet pressure depends on the pressure of the H_2 tank, but it is considered to be constant for this model.

The model can be considered as a black box represented in the Figure 4.7 having the following characteristics. As inputs, the water pump has the current temperature of the water tank and the water mass flow rate demanded by the electrolysis to produce Hydrogen. The parameters that were exposed above. And as outputs, the power consumption of the pump at each time, the energy

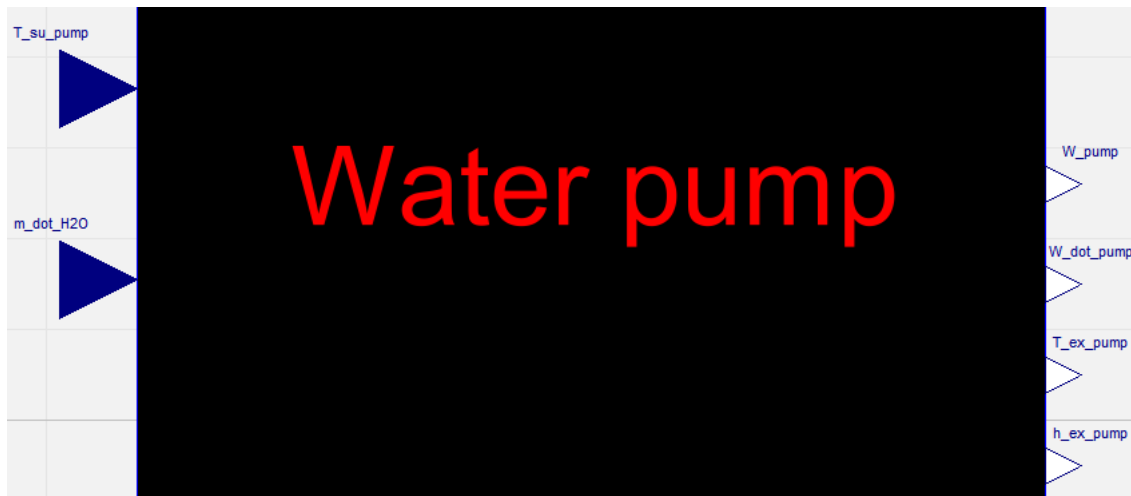consumption in all the simulation, the outlet temperature and the outlet specific enthalpy at each time.

Figure 4.7: Representation of the water pump's diagram with inputs and outputs.

The equations that define the water pump were based on thermodynamics knowledge.

Knowing the inlet pressure and temperature and the exhaust pressure, the inlet enthalpy and entropy and the exhaust isentropic enthalpy can be obtained. Then, by the definition of the isentropic efficiency exhaust enthalpy can be found. Finally, using these parameters and the hydrogen mass flow rate, the work produced by the pump and the energy consumption can be calculated. This explanation is described in the followings equations.

The definition of the isentropic efficiency of a pump is:

$$\eta_s = \frac{w_{s_{pump}}}{w_{pump}} = \frac{h_{ex_{s_{pump}}} - h_{su_{pump}}}{h_{ex_{pump}} - h_{su_{pump}}}$$
Equation WP1

where $w_{s_{pump}}$ and w_{pump} are respectively the isentropic specific work and the specific work realised by the pump; and the exhaust temperature can be obtained by the knowledge of the exhaust pressure and enthalpy. Then, the work produced is defined as:

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$$\dot{W}_{pump} = \dot{m}_{H_2O} * w_{pump} \qquad \text{Equation WP2}$$

Finally, the energy consumed can be calculated by the integration of the Equation WP_2 on the simulation time.

4.6. Hydrogen compressor

After performing the analysis of the different compressors technologies and taking into account the characteristics of the system, the best option could be a non-mechanical compressor because the flow mass ratio of hydrogen is not too high, so the efficiency would be better. However, the time required to realise a model for this kind of compressor is longer than for a volumetric hydrogen compressor.

The principal hypothesis that has been done to this model takes into account a constant value of the isentropic efficiency. The value chosen was 50%, for security is less than the value mentioned in [40]. The model was made in the Engineering Equation Solver (EES) and compared with the water pump.

The definition of the isentropic efficiency is presented as:

$$\eta_s = \frac{w_{s_{compressor}}}{w_{compressor}} = \frac{h_{ex_{s_{compressor}}} - h_{su_{compressor}}}{h_{ex_{compressor}} - h_{su_{compressor}}} \qquad \text{Equation H21}$$

Knowing the inlet pressure and temperature of the compressor and the outlet pressure desired, the specific works (isentropic and 'real' ($w_{s_{compressor}}$ and $w_{compressor}$ respectively)) can be obtained.

Finally, the work produced by the compressor is:

$$\dot{W}_{compressor} = \dot{m}_{H_2} * w_{compressor} \qquad \text{Equation H22}$$

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4.7. Expander

The expander model is represented in Figure 4.8. It is composed of an expander (micro-turbine) and a valve. As inputs the expander system has the temperature of the hydrogen tank and the hydrogen mass flow rate demanded by the fuel cell. As outputs, the mechanical expander has the isentropic efficiency and the pressures that are fixed by the hydrogen tank (inlet) and by the minimal temperature that it is needed at the exhaust of the valve. As outputs: the electrical power produced, the exhaust temperature and enthalpy; the last one will be the input of the valve. The parameter that characterises this valve is the outlet pressure required. As output the valve has the exhaust temperature that is the minimal temperature necessary in the fuel cell.
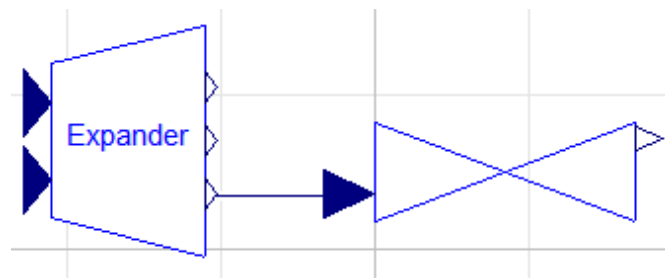
Figure 4.8: Representation of the expander system.

The isentropic efficiency of the expander is defined as follow:

$$\eta_{s_{exp}} = \frac{w_{exp}}{w_{s_{exp}}} = \frac{h_{su_{exp}} - h_{ex_{exp}}}{h_{su_{exp}} - h_{ex_{s_{exp}}}}$$

Equation Ex1

And the work produced by the mechanical expander is:

$$\dot{W}_{exp} = \dot{m}_{H_2} * w_{exp}$$

Equation Ex2

Once the work produced calculated, the energy produced can be obtained doing the integration on the simulation time of the Equation Ex2.

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5. Results of the simulations of hydrogen-based energy storage systems integrated into buildings

Using the sub-models explained in section 4, the complete system is realised and represented in Figure 5.1.

Figure 5.1: Diagram of the system
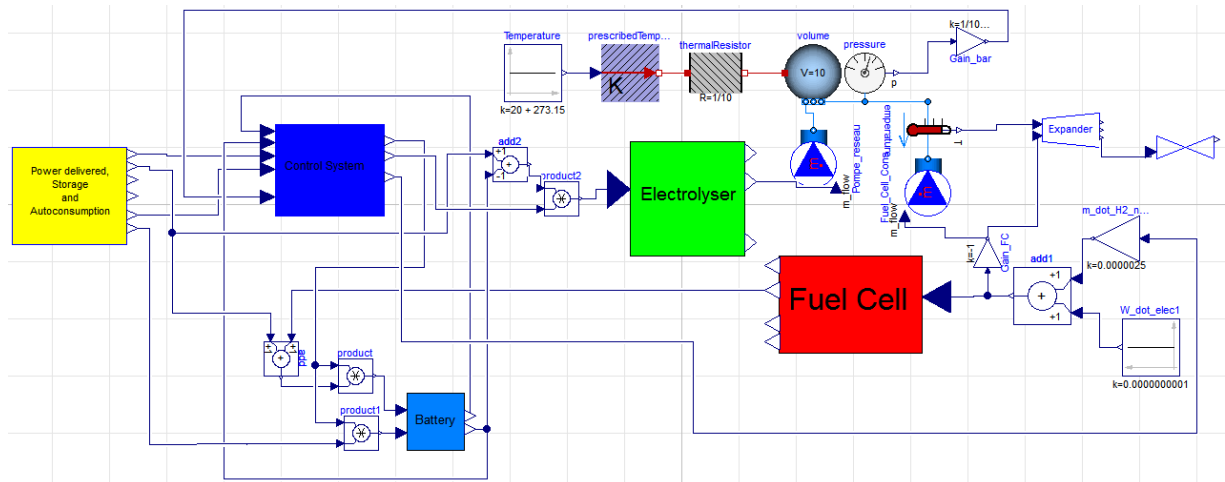
The control system realised regulates the charge and discharge of the battery; and the production and consumption of H_2. The inputs of the control system are the SOC of the battery, the power demanded to the battery, the total consumption of the residential building, the PV production and the pressure of the storage volume.

One of the main objective of the project is the study of energy flexibility in residential buildings. Because a lot of parameters can be modified on the system, the analysis was realised considering three parameters and various hypothesis:

- The storage volume of H_2 (V_{sto}) having values of 2, 6 and 10 m³.
- The surface of the PV panels PV_{m^2} with values of 15, 20 and 40 m².
- The capacity of the battery C_{bat} with values of 7, 13.2 and 20 kWh.
- The H_2 tank is supposed to be charged at the beginning of the year (70 bar).
- The battery is supposed to be at 50 % of its capacity at the beginning of the year.
- The capacity given by the manufacturer is the useful capacity so, the depth of charge is 100%.

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- Minimal pressure in the H_2 tank of 5 bar is required, so the tank is never completely empty.

The hydrogen compressor was modelled and simulated for the following conditions: T_{su} = 40ºC, P_{su} = 70 bar, P_{ex} = 200 bar and the maximum mass flow rate of H_2 that can be obtained (PV_{m^2} = 40 m^2 and C_{bat} = 7 kWh) equal to 2.01507*10^{-5} kg/s.

The power needed for the compression work was 67,83 [W] and the cylinder volume is 0.07736 cm^3. This kind of compressor was not found. Nevertheless, the compressor wasn't included in all the simulations because it was estimated that 70 bar will be enough as storage pressure. The pressure is realised by the water pump and the power consume is 0.63 W and the cylinder volume is 0.002025 cm^3. The cylinder volume of the compressor and the water pump are calculated at 50 Hz.

It must be note that the total electrical consumption of the residential building that is considered in this project is ~3000 kWh/year, and the PV production is presented in table 5.1.

Table 5.1: PV energy production in 1 year and PV power (ANNEXE) at different surfaces.

	15 m^2 of PV	20 m^2 of PV	40 m^2 of PV
Energy produced [kWh/year]	2250	3000	6000
Pic Power range [W$_p$]	3970 – 4200	5300 – 5600	10600 – 11200

The simulation is realised for a time of one year. Figure 5.2 represents the different power that appears in the system: the power delivered by the PV panels (orange), the battery (red) and fuel cell (violet), and the power consumed by the residential building (dark blue), the battery (light blue) and the electrolyser (green).

It can be observed in Figure 5.2 that the electrical consumption is maintained in the range between 0 and 1000 W with some pics outside this range. The power production of the PV is bigger in summer than in winter, as expected. For this reason almost the entire production of hydrogen (produced by the electrolyser) is in summer. Also, for the same reason, the production of electrical energy using the fuel cell to charge the battery is outside the summer range.
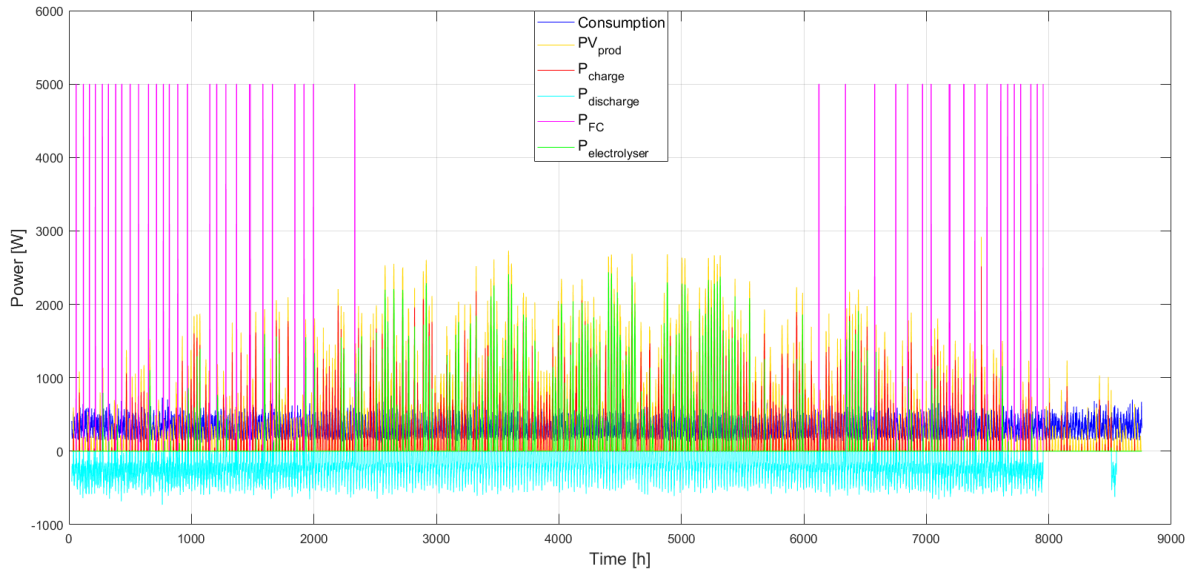
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Figure 5.2: Representation of the electrical power consumed by the residential building in one year, the power produced by the PV panels, the power used to charge and demanded to discharge the battery, the power delivered by the fuel cell and the power provided to the electrolyser. The capacity of the battery used is 13.2 kWh, the surface of PV panels is 20 m^2 and the tank volume is 6 m^3.

Figure 5.3 represents the state of charge (SOC) of the battery using the same conditions as for the simulation of Figure 5.2.

A comparison between Figures 5.2 and 5.3 can be realised. It can be observed in Figure 5.3 that in summer the battery is never completely discharged. At the beginning of the year the charge is faster due to the assumption that the hydrogen storage tank is full, so, more H$_2$ can be released to produce electricity using the fuel cell. At the end of the year the battery charges slowly because the H$_2$ tank is empty and the charge is only due to the surplus power production of PV panels.

Two days, a typical warm day and a typical cold day are considered to observe in more details how the system behaviours under these circumstances.
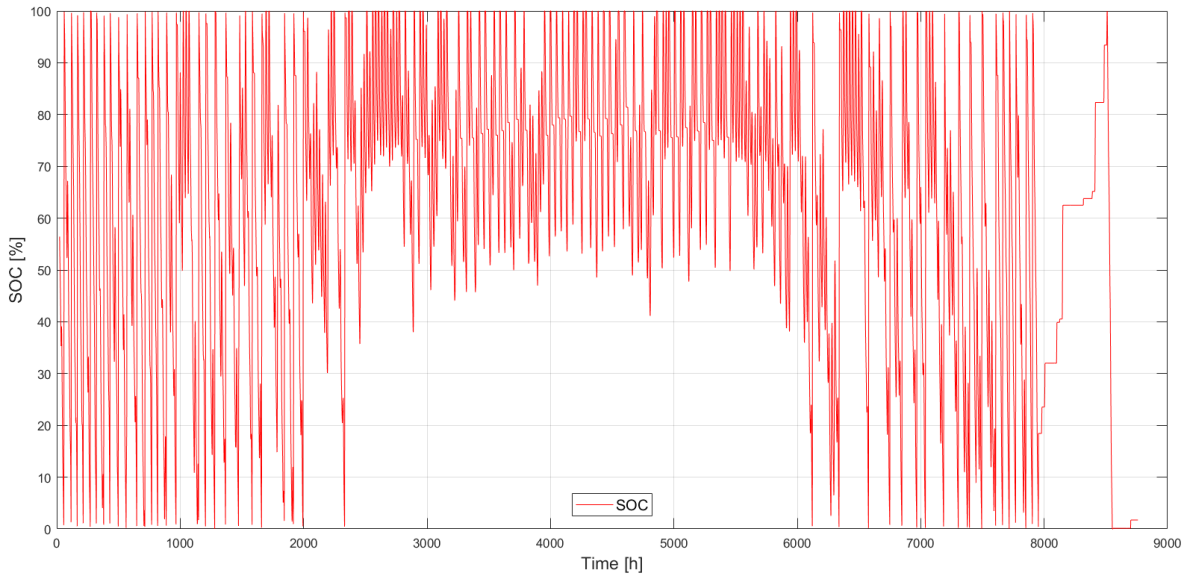
Figure 5.3: Representation of SOC of the battery with a capacity of 13.2 kWh for a tank volume of 6 m^3 and a PV surface of 20 m^2.

The Figure 5.4 summarises a warm day presenting the building consumption, the PV panels production, the power gives to the battery on charge mode and the power demanded to the battery in discharge mode, the power given to the electrolyser and the power demanded to the fuel cell to recharge the battery.

Figure 5.4: Representation of a typical warm day (from the 3rd of July to 4th of July). It was considered a PV surface of 20 m^2, a battery of 13.2 kWh and a H_2 storage volume of 6 m^3.

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Figure 5.4 can be related with Figure 5.5 to understand how the energy is crossing the system.
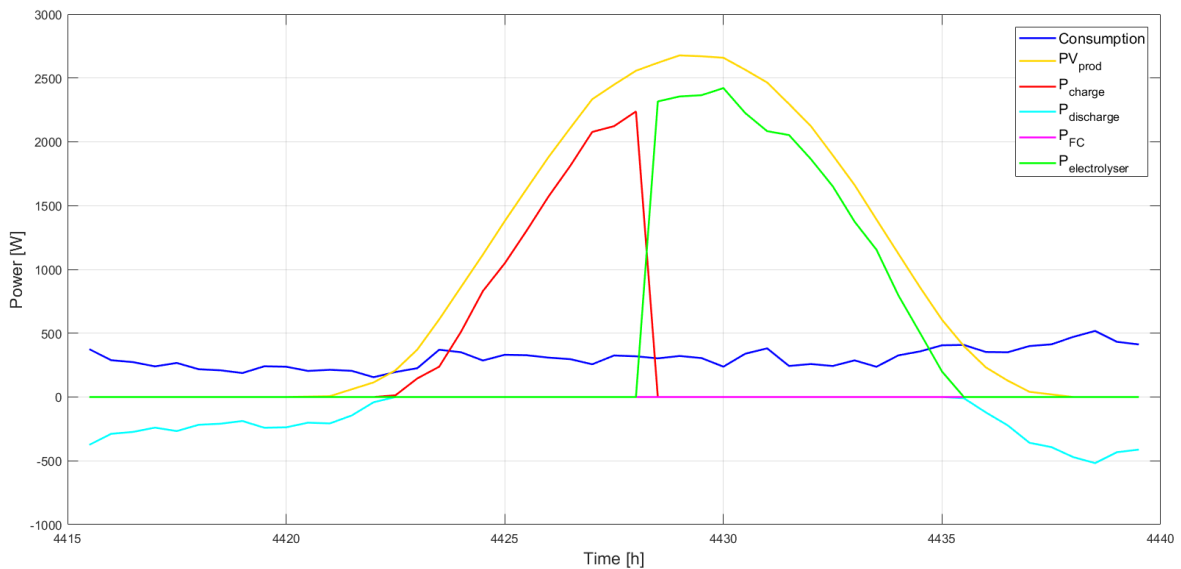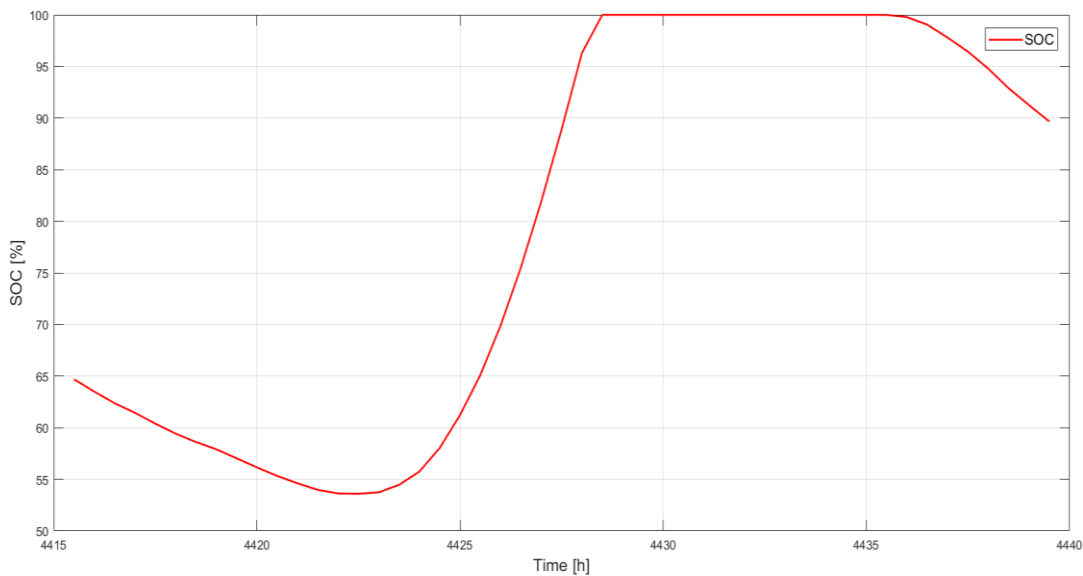

Figure 5.5: Representation of the state of charge (SOC) of the battery.

It can be observed at the beginning of the day (hour 4416 of the year that is 0:00 of the 184 day of the year) that the battery is providing the power demanded by the residential building. Consequently, the battery is in mode discharge. When the sun is rising (~5:00) the power produced by the PV panels is still not enough to satisfy the demand so, the battery is in continuous process to discharge, but slower than previously. When the PV power produced is bigger than the demand, the battery starts to charge. Once the battery is reaching the SOC of 100 %, the electrolyser starts to receive the remaining power between the power of the demand and PV panels. Two conditions happen on the system for the power received by the electrolyser: the electrolyser receives power, and consequently generates H_2, until the pressure in the storage tank achieve the maximum pressure delivered by the electrolyser or until (the ones that occur in this occasion) the power delivered by the PV panels is not enough to satisfy the demand. When this happens, the battery starts to discharge providing the amount of power required by the residential building. At this moment it is not covered by the PV panels and the cycle starts again. It should be added that the fuel cell is in off mode. This occurs because of two operational conditions. The first one is that the fuel cell will provide the energy to the battery only if the SOC is 0 % (the datasheet of the battery give the depth of the

charge (100%), in reality the batteries are never completely discharged in order not to damage the battery). The second is that the H_2 tank must have enough H_2 inside to provide to the fuel cell.

The Figure 5.6 summarise a typical cold day with the same legend of the Figure 5.4.
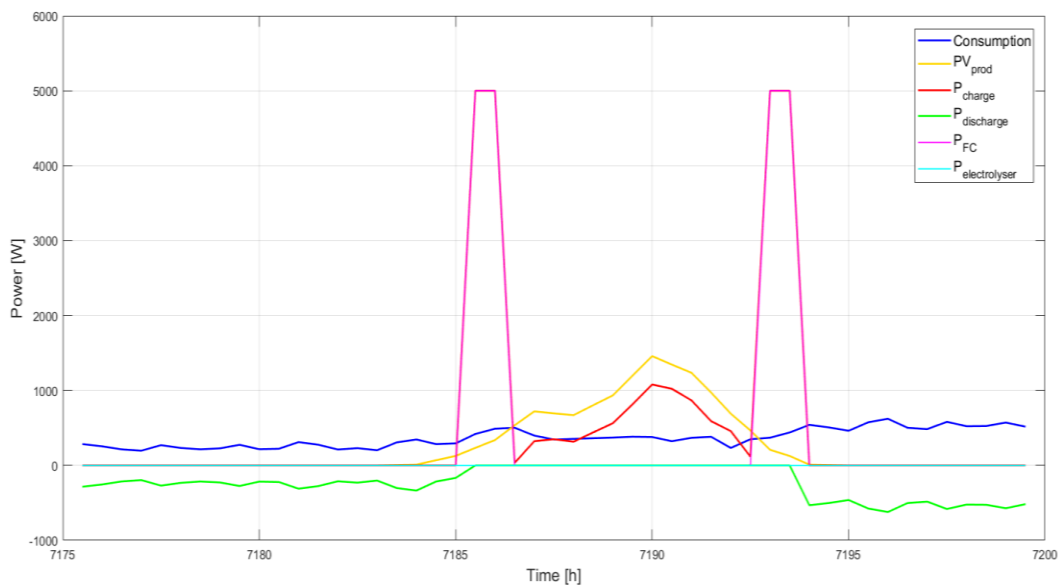
Figure 5.6: Representation of a typical cold day (from the 26th of October to 27th of October). It was considered a PV surface of 20 m^2, a battery of 13.2 kWh and a H$_2$ storage volume of 6 m^3.

Figure 5.6 can be related with Figure 5.7 to understand how the energy is crossing the system.

As illustrated, at the beginning of the day (0:00) the battery is providing the power required by the residential building until the depth of charge is 0%. At this moment, the fuel cell provides the power required for the battery to be charged until the PV panels power is bigger than the consumption. Then, the fuel cell turns off and the battery is charged only by the PV panels until the power required by the residential building is the same as the power produced. The end of the charged is done by the FC. Once the battery is completely charged, it starts to discharge providing the power required by the system.

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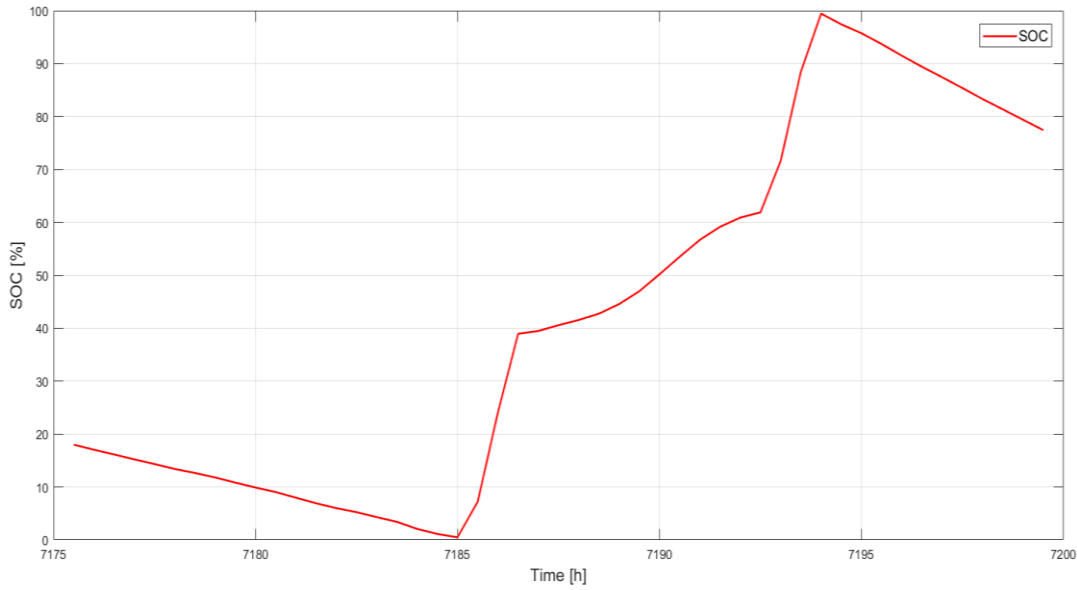
Figure 5.7: *Representation of the state of charge (SOC) of the battery.*

Changing the three parameters presented at the beginning of the section (H$_2$ storage volume, capacity of the battery and surface of the PV panels) 27 possible simulations were generated. Following, three case studies are presented on which one of the three parameters is changed while the other two remain fixed. Also, it should be noted that, for reasons of compilation of Modelica, the **Equation Elect1** has been modified as follows:

$$V_{TP_{cell}} = 0.7551 * I_{cm^2} + 1.572 \qquad \text{Equation 5.1}$$

Consequently, the behaviour of the electrolyser will not be the same. The Equations 5.2 and 5.3 represent an additional way to define the electrolyser and respectively the fuel cell efficiency.

$$\eta_{electrolyser} = \frac{m_{H_2 produced} * LHV_{H_2}}{W_{electrolyser}} \qquad \text{Equation 5.2}$$

$$\eta_{FC} = \frac{m_{H_2 used} * LHV_{H_2}}{W_{FC}} \qquad \text{Equation 5.3}$$

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Where $m_{H_2produced}$ and m_{H_2used} are respectively the H$_2$ mass produced and consume, the LHV_{H_2} is the Low Heating Value of Hydrogen (120000 kJ/kg), W$_{electrolyser}$ is the energy provided to the electrolyser and W$_{FC}$ the energy produced by the fuel cell.

The three cases proposed, analyse the degree of auto-consumption and the degree of the demanded covered. Then, the pressure in the H$_2$ tank jointly the H$_2$ mass production and consumption is analysed.

First, it should be defined what represents these degrees. The auto-consumption or self-consumption degree of the local production γ_s (presented in Equation 5.4), represents the percentage of the local production of electric energy consumed instantaneously by the building. The demand covered degree γ_d (presented in Equation 5.5), represents the percentage of the building electrical demand that can be covered instantaneously by the local production of electric energy.

$$\gamma_s = \frac{\sum \min(\dot{W}_{cons}, \dot{W}_{Prod})}{\sum \dot{W}_{Prod}}$$

Equation 5.4

$$\gamma_d = \frac{\sum \min(\dot{W}_{cons}, \dot{W}_{Prod})}{\sum \dot{W}_{cons}}$$

Equation 5.5

Where $\dot{W}_{cons}$ is the total electrical power consumption of the building and $\dot{W}_{Prod}$ is the total local electrical power production [41].

A base case is presented in Figure 5.8 analysing the absence of the hydrogen production or store and the use of electrical batteries in a residential building.

As can be observed, γ_s decreases with the increase of the surface of the installed PV panels. This is expected because if more power is installed at the same time more power will be provided to the grid if it is not consumed. On the other hand, γ_d decreases as the surface of PV panels increases, but it can be observed that it has an asymptote trend. The optimal point will be the one that gives the higher γ_s. Usually, an elevate γ_d denotes a decrease of costs because more demand is covered instantaneously by the local production, so, less demand must be covered by the grid.
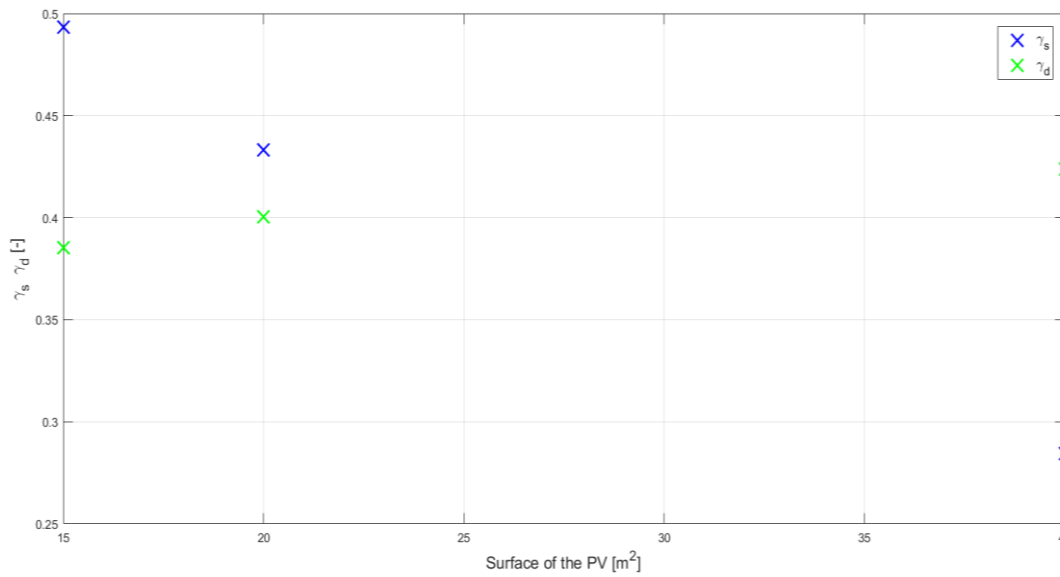
Figure 5.8: Representation of the auto-consumption and demand covered degree for a year of simulation changing the PV panels surface.

The following cases will be compared to the base case to observe if these significant values change and how they change.

The case 1 is presented in Figures 5.9 and 5.10 and analyses the behaviour of the residential building with the presence of a system with a variable volume of H_2 tank, a fixed capacity of battery and a fixed surface of PV panels.

Figure 5.9: Representation of γ_s and γ_d for different volumes of H_2 tanks, using a battery capacity of 13.2 kWh (as the battery shown in the ANNEXE) and a PV panels surface of 20 m^2.

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As shown, using a H$_2$ tank of 2 m^3 γ_s and γ_d are increased around the double of the previous value. The increase of γ_s is due to the opportunity to store the energy produced by the PV panels. In another point of view, the surplus of energy provi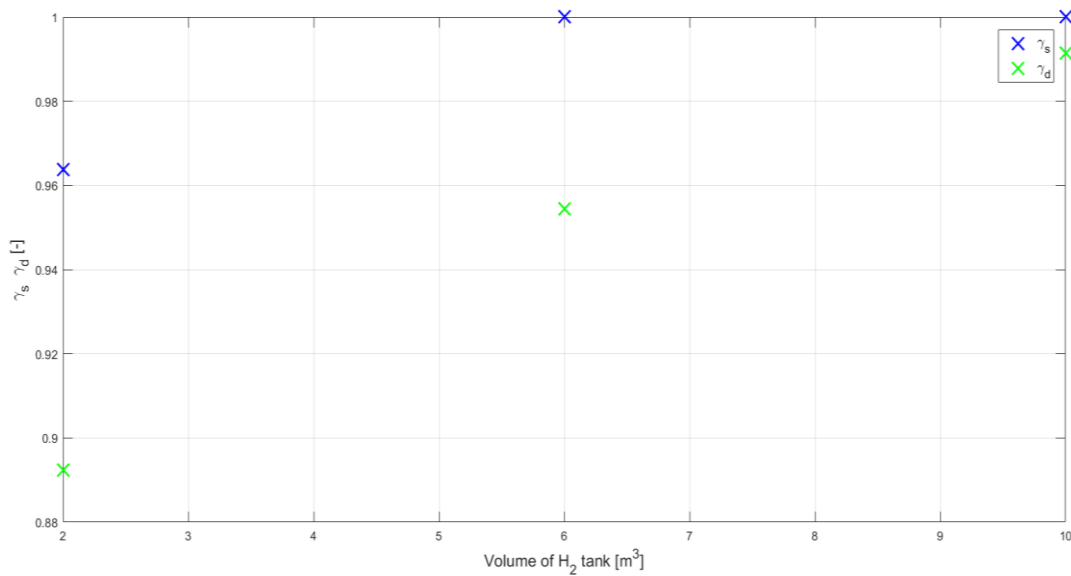ded by the PV panels is consumed instantaneously by the battery and occasional by the electrolyser to produce hydrogen instead of sending this surplus to the grid. And the increase of γ_d is due to the augmentation of the energy that can be delivered, not by the PV panels (because compared to the base case is the same) but thanks to the energy that can be provided by the battery and the FC.

Figure 5.10 represents the variation of pressure in the hydrogen storage tank and the mass of hydrogen produced and consumed in a year.
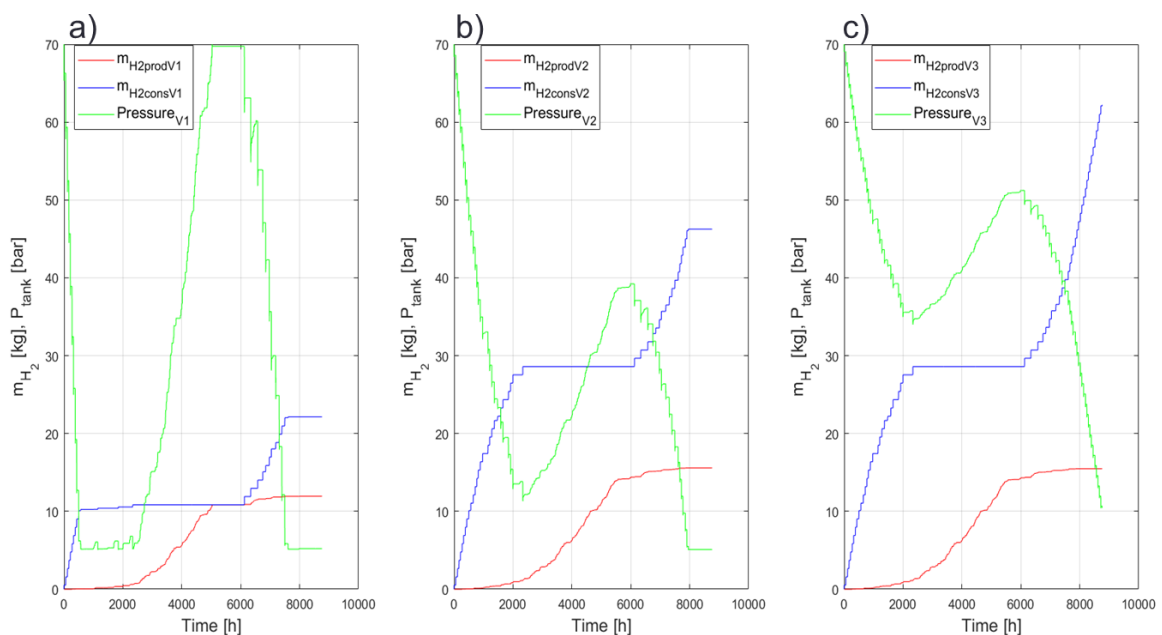
Figure 5.10: Representation of variation of H$_2$ pressure in the tank, the H$_2$ mass production and consumption for different size of tanks: **a)** 2 m^3; **b)** 6 m^3; and **c)** 10 m^3.

It can be observed in Figure 5.9 that γ_s increases with the dimension of the tank because more energy can be stored and compared to Figure 5.10 the pressure in the tank achieve its maximum for a volume of 2 m^3. This means that H$_2$ cannot be produced in more

quantity as can be observed when the volume of the tank is increased in Figures 5.10 b) and c).

The Figure 5.10 gives more information about the total consumption in the year. If a comparison is realized between a), b) and c), it can be observed that in all cases the consumption of H_2 is bigger than the production in all year. This can be possible because of the initial value of hydrogen pressure. In a) and b) it can be affirmed that the tank arrives until the minimal value of pressure, this means that hydrogen cannot be provided anymore. Figure 5.10 c) shows a bigger consumption even if the production is the same. That is possible due to the fact that for the same initial hypothesis of pressure there is a bigger amount of H_2 in 10 m^3 than in 6 m^3. Another statement is that the variation of pressure is slower when the size of the tank increases.

The case 2 is presented in Figures 5.11 and 5.12 and analyses the behaviour of the residential building with the presence of a system with a fixed volume of H_2 tank, a variable capacity of battery and a fixed surface of PV panels.

It can be observed in Figure 5.11 that γ_s is not influenced by the capacity of the battery. This happens because the volume of 6 m^3 is large enough to store the energy with the small capacity of the battery. However, γ_d increases due to the fact that more energy can be provided instantaneously. However, this increase is slow because the H_2 tank is large enough to produce the energy that the battery cannot.

When the capacity of the battery increases, the production of H_2 decreases. This effect can be observed in Figure 5.12.

As shown in Figure 5.12 more the capacity of the battery increases, less hydrogen is produced and consumed. This happens because more energy can be absorbed by the battery. It can be observed that pressure increases less even if there is more H_2 produced. This is because at low battery capacity the complete discharge will be faster so, the battery will need to be charged more frequently by the FC. Consequently, more H_2 will be consumed. Also, it is because the volume of H_2 tank is 6 m^3. In Figure 5.10 it was shown that with a capacity of 13.2 kWh the pressure reaches the saturation level

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with a H_2 tank of 2 m^3. Consequently, if the capacity of the battery and the volume of tank decrease, the pressure will increase faster because H_2 is produced.
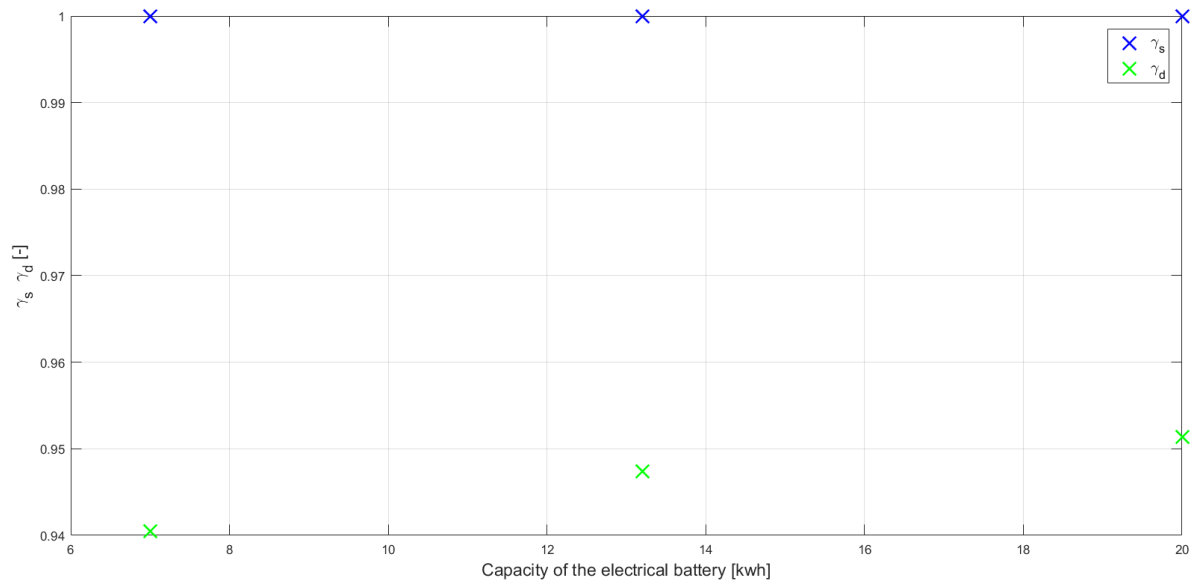
Figure 5.11: Representation of γ_s and γ_d for a fixed volume of H_2 tanks at 6 m^3, using different battery capacity (7, 13.2 and 20 kWh) and a PV panels surface of 20 m^2.

Figure 5.12: Representation of variation of H_2 pressure in the tank, the H_2 mass production and consumption for different size of battery: **a)** 7 kWh; **b)** 13.2 kWh; and **c)** 20 kWh.

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The case 3 is presented in Figures 5.13 and 5.14 and analyses the behaviour of the residential building with the presence of a system with a fixed volume of H_2 tank, a fixed capacity of battery and a variable surface of PV panels.
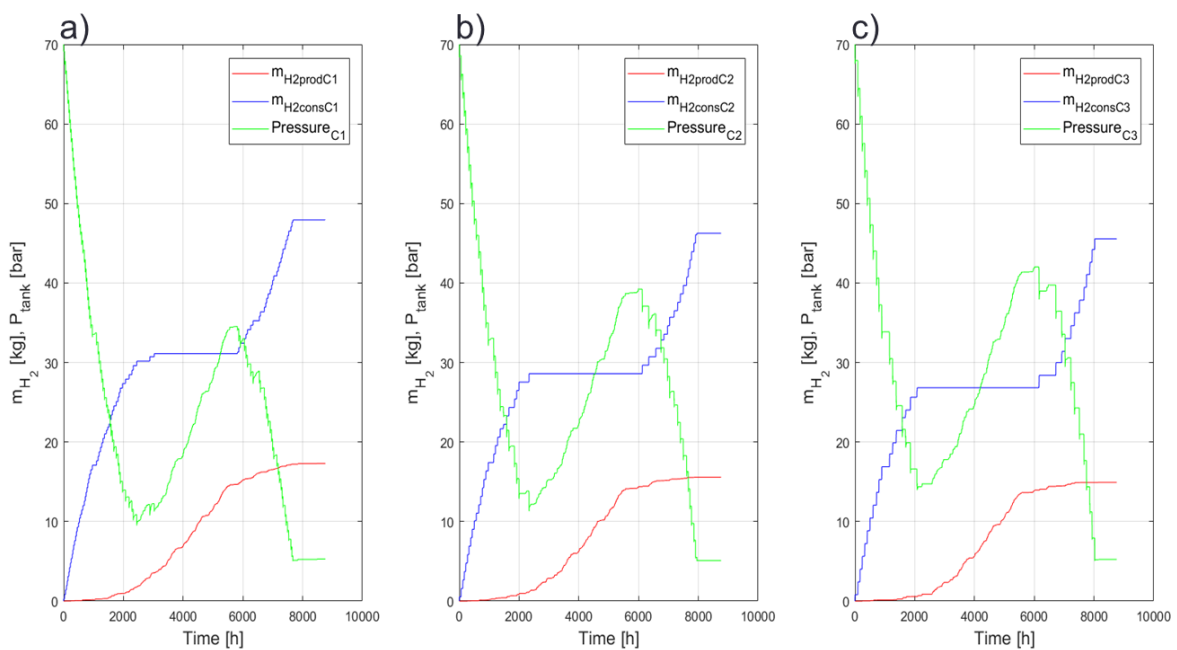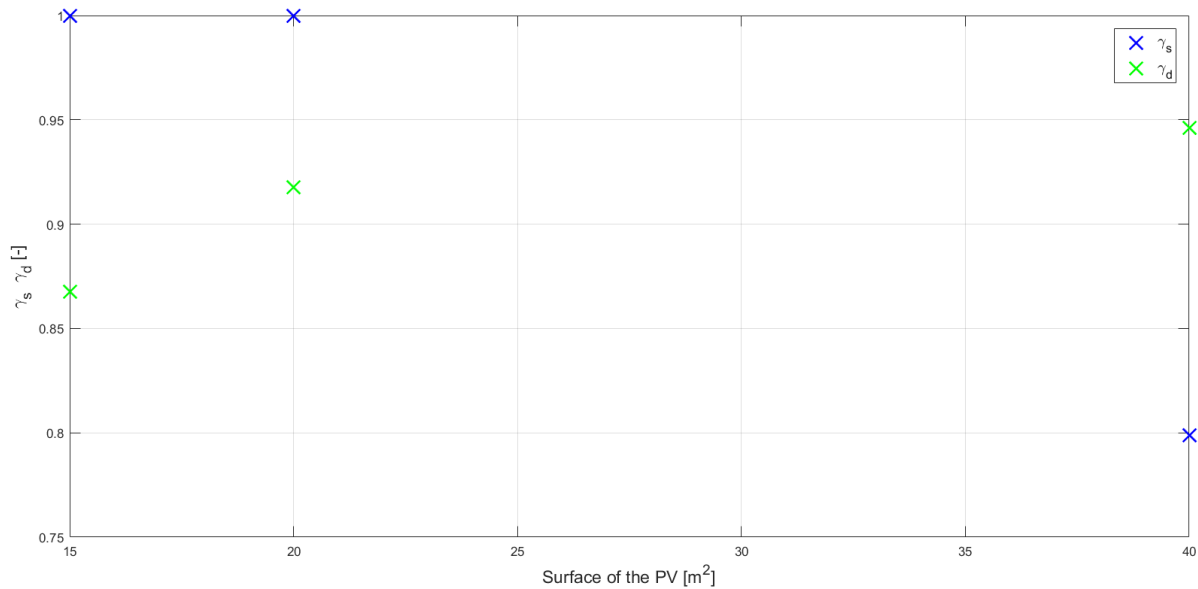

Figure 5.13: Representation of γ_s and γ_d for a fixed volume of H_2 tanks at 6 m³, using a battery with a capacity of 13.2 kWh and a variable PV panels surface of 15, 20 and 40 m².

It can be observed in Figure 5.13 that γ_s is not affected with 15 and 20 m² because all the energy produced by the PV panels is consumed by the system. But with 40 m² γ_s decreases because the capability of the system to consume the power generated decreases. On the other hand, γ_d increases because more power is available to respond the instantaneous demand. It must be noted that γ_d has an asymptotic trend.

Figure 5.14 can be compared to 5.13 to do a better explanation of why γ_s decreases. It can be observed that with the power generated by the 15 m² of PV panels is not enough to generate H_2 and maintain a pressure in the tank. But, γ_s is 1 because all the power produce can be absorbed by the system. When the surface is 20 m², there is an augmentation of H_2 production so, an increase also in the consumption. Finally, when the surface is 40 m² the storage tank reaches the saturation at 70 bar. So, not more hydrogen can be produced. Knowing that the SOC is 100% due to the quickly charge of

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the battery, the power produce by the PV panels is not consume and it is rejected to the grid. For this reason, γ_s decreases.
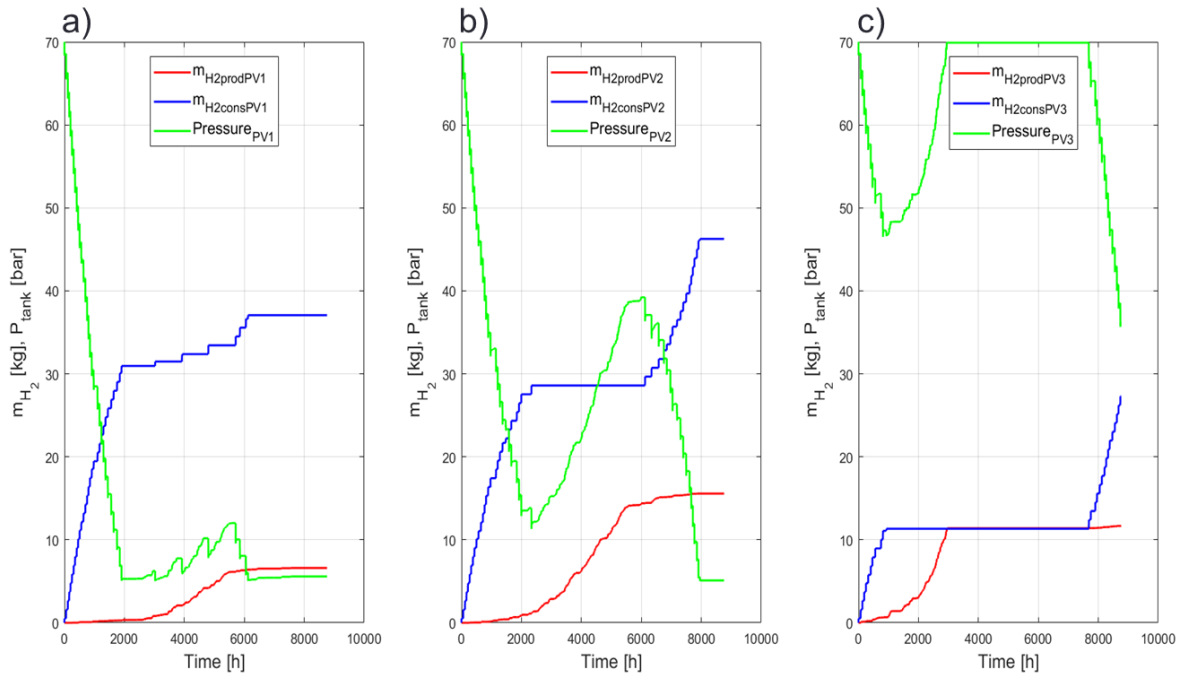
Figure 5.14: Representation of variation of H_2 pressure in the tank, the H_2 mass production and consumption for different surface of PV panels: **a)** 15 m²; **b)** 20 m²; and **c)** 40 m².

Comparing the three cases explained above, it can be observed that there exists an optimal volume of H_2 fixing at the nominal surface of the PV panels (20 m²) and the typical capacity of the battery that exist in the market (13.2 kWh). This optimal is located between 2 and 6 m^3 of tank. The main issue is that the system depends on the initialisation conditions, so the time of simulation must be increased to 2 years.

In Figure 5.15 is represented the analyse of the behaviour of the residential building with the presence of a system with a variable volume of H_2 tank, a fixed capacity of battery and a variable surface of PV panels.

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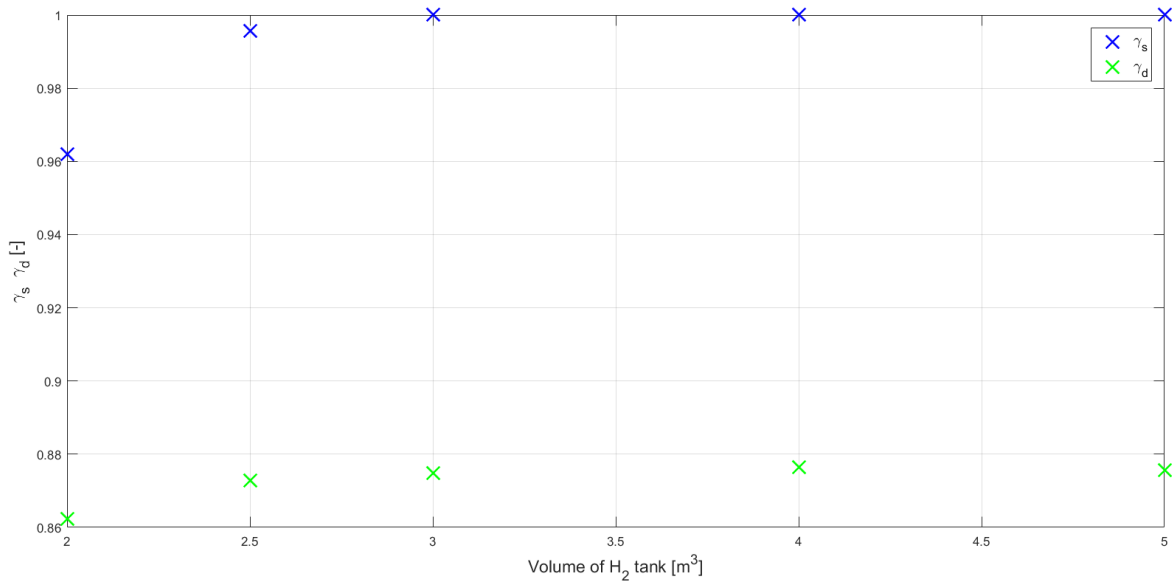
Figure 5.15: Representation of γ_s and γ_d for different volumes of H$_2$ tanks (2, 2.5, 3, 4 and 5 m^3) using a battery capacity of 13.2 kWh and a PV panels surface of 20 m^2.

It can be observed in Figure 5.15, that γ_s and γ_d increase with the volume of the tank and both have an asymptote trend.

Comparing Figure 5.15 and 5.16 it can be observed that pressure reaches the saturation level at 70 bar for the Figure 5.16.a) and 5.16.b). The optimal value of tank volume would be the one that permits the inside pressure to be near saturation but without reaching it. γ_s reaches the value of 1 at 3 m^3 so, this will be the final volume chosen for the H$_2$ storage tank volume. If a specific value wants is required a further study will be needed.

Figure 5.16 demonstrates that the consumption of H$_2$ as expected cannot be bigger than the production. In fact, it is the same because in all these cases the pressure in the tank starts and finishes at the same value of 5 bar. It can be observed, that the production of H$_2$ increases with volume until the pressure does not reach anymore the saturation.

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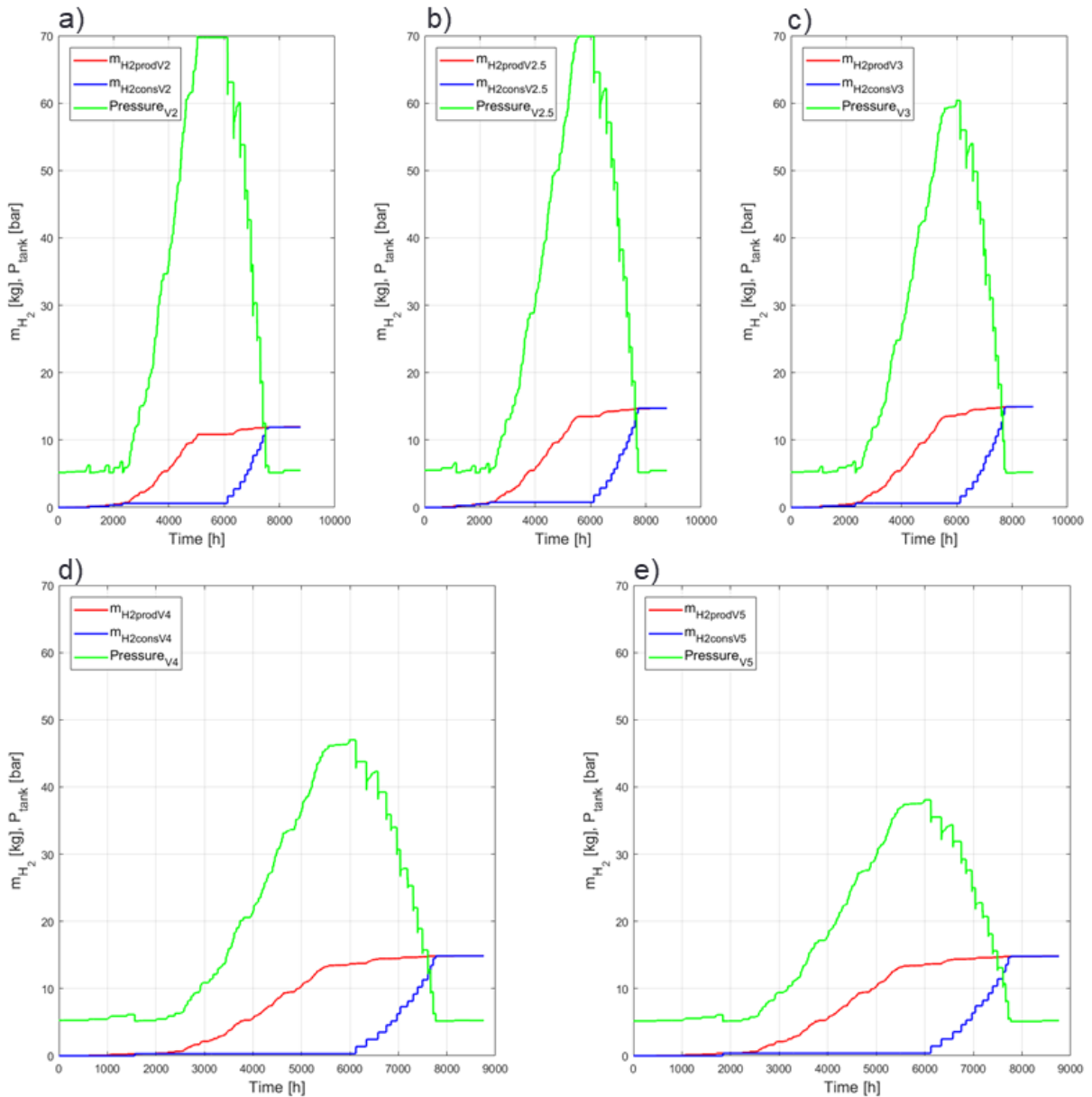
1Figure 5.16: Representation for the 2nd year of simulation of variation of H$_2$ pressure in the tank, the H$_2$ mass production and consumption for different size of tanks: **a)** 2 m^3; **b)** 2.5 m^3; **c)** 3 m^3; **d)** 4 m^3; and **e)** 5 m^3.

As previously presented the energy generated by the PV panels is 3000 kWh per year. The instantaneously energy consumed by the residential building is 1019.03 kWh and the remaining energy is sent to the storage system. The energy recovered from the storage system is 1270.52 kWh.

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The total energy stored in the battery (W_{sto}), the total production and consumption of H_2, and the fuel cell and electrolyser efficiency for the last case presented are summarized in Table 5.2.

Table 5.2: Results of the storage system.

$W_{sto}\ [kWh]$	1195.78
$\eta_{bat}\ [\%]$	89
$m_{H_2 produced}\ [kg]$	14,82
$m_{H_2 used}\ [kg]$	15
$W_{electrolyser}[kWh]$	785.19
$W_{FC}\ [kWh]$	206.28
$\eta_{electrolyser}\ [\%]$	63
$\eta_{FC}\ [\%]$	42

Finally, the energy demand covered by the system is 2289.55 kWh so, approximately the 76.3 % of the electrical demand is covered.

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6. Conclusions and perspectives

In this project a hydrogen-based energy storage system has been modelled for the investigation of the energy flexibility of a residential building.

This kind of system would be interesting to implement in order to reduce the use of fossil fuels for energy production since, this process has a huge impact on CO_2 footprint.

The developed system gave interesting results considering the simplicity of the model and the hypotheses formulated for each sub-model.

It was shown that the consumption of H_2 is always bigger than the production. The hypotheses for the values chosen to initiate the simulation have an impact on the variability of the results for one year. Consequently, the simulation time must be increased to two years.

The optimal volume for the simulations of one year was found to be between 2 and 6 m^3 fixing the other two parameters at the nominal values of 13.2 kWh for the capacity of the battery and 20 m^2 for the surface of PV panels.

A first conclusion can be obtained for the last results obtained for the simulation of 2 years.

A sizing of the installed power of PV panels is usually compared to the energy that must be delivered to satisfy the energy demand. In this project, as previously clarified, the total electric energy demanded by the residential building in a year is 2888.55 kWh so, approximately 3000 kWh. The energy produced by m^2 of PV panel is 150.47 kWh so, approximately 150 kWh. That gives a nominal surface of the PV panels installed of 20 m^2.

The fuel cell chosen for this project is the one that was already bought by the electrochemical laboratory of the University of Liège. It delivers 5 kW_{elec} so, a battery which can support the power deliver by the FC was needed. For this reason,

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the battery found in the market with these characteristics was the battery of TESLA (datasheet shown in ANNEXE).

Finally, the electrolyser was modelled using an experimental curve obtained in [27].

The optimal volume of H_2 storage tank obtained, with the last results, has a value between 2.5 and 3 m^3. This value is interesting because even if the dimension can be found easily in the market, 3 m^3 is not an exorbitant volume for a residential building.

Finally, after all the simulations realised, it can be concluded that technically the project can be performed and a hybrid storage system of electrical batteries (with 13.2 kWh of capacity) and H_2 tanks (with 3 m^3 of volume) seems to be a good way to further improve the self-consumption (γ_s of 1) and covered demand degree (γ_d bigger than 0.87). However, further studies must be done in order to confirm these affirmations.

To obtain better results that reflect the reality of a system of these characteristics each sub-model will have to be more elaborated. That needs more time and knowledge. Considering, each part of the project some perspectives can be done.

First, a detail study of the local climate and geographical conditions must be done. This kind of study is time consuming. Once this study is realised, the source of the electrical energy can be selected accordingly (wind turbines for windy zones, or small hydroelectric turbines for river zones, etc). A comparison between using only the electricity of the grid; a mix using renewable energies and the grid; and using only renewable energy should be made in the future to study the economical aspect between them.

A comparison with a system that considers the electrolyser that are not under pressure must be equally done. In this manner, to know if the additional power that must be delivered to produce the electrolysis is insignificant or must be considered.

Finally, as long as the technology is under developing, make a precisely model will be easier because more details about them will be appearing. The technological

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advances have been evolving more in the last 10 years [42] and the cost is decreasing. For example, the hydrogen fuel cell of the laboratory since its project was developed until they finally bought the NEDSTACK FC the price decreased more than 20%. Consequently, the techno-economic analysis done by [43] in the year that was done, now would have some different results and conclusions. In my opinion, better results could be obtained due to the advances in the technology.

This work serves not only as an introduction for a further study but also for the obtention of concrete results: a specific value of volume of H_2 tank, a specific value of PV surface needed, a good degree of self-consumption and a relatively good performance in general.

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7. References

[1] P. Nejat, F. Jomehzadeh, M.M. Taheri, M. Gohari, M.Z. Muhd, A global review of energy consumption, CO2emissions and policy in the residential sector (with an overview of the top ten CO2emitting countries), Renew. Sustain. Energy Rev. 43 (2015) 843–862. doi:10.1016/j.rser.2014.11.066.

[2] BP, Statistical Review of World Energy, 2016. doi:10.1016/j.egypro.2013.06.172.

[3] T.A. Boden, G. Marland, R.J. Andres, Global, Regional and National Fossil-Fuel CO2 Emissions., 2015. doi:10334/CDIAC/00001_V2015.

[4] H. Rodhe, A comparison of the contribution of various gases to the greenhouse effect., Science (80-.). 248 (1990) 1217–1219. doi:10.1126/science.248.4960.1217.

[5] M. Channdel, E. Williams, Synthetic Natural Gas (SNG): Technology, Environmental Implications, and Economics, Work. Pap. (2009).

[6] Battery Comparison of Energy Density - Cylindrical and Prismatic Cells, (n.d.). http://www.epectec.com/batteries/cell-comparison.html (accessed April 4, 2018).

[7] N. Job, Safety issues in hydrogen handling, in: U. of Liege (Ed.), Electrochem. Energy Convers. Storage Syst., Liege, 2018. doi:10.1021/ar200215t.

[8] M. Harada, T. Ichikawa, H. Takagi, H. Uchida, Building a hydrogen infrastructure in Japan, Compend. Hydrog. Energy. (2016) 321–335. doi:10.1016/B978-1-78242-364-5.00014-2.

[9] J. Lu, A. Zahedi, C. Yang, M. Wang, B. Peng, Building the hydrogen economy in China: Drivers, resources and technologies, Renew. Sustain. Energy Rev. 23 (2013) 543–556. doi:10.1016/j.rser.2013.02.042.

[10] M. Steen, Building a hydrogen infrastructure in the EU, Compend. Hydrog. Energy. (2016) 267–292. doi:10.1016/B978-1-78242-364-5.00012-9.

[11] N. Job, Fuel cells: fuel management, in: Electrochem. Energy Convers. Storage, University of Liege, Liege, 2018.

[12] C.M. Kalamaras, A.M. Efstathiou, Hydrogen Production Technologies: Current State and Future Developments, Conf. Pap. Energy. 2013 (2013) 1–9. doi:10.1155/2013/690627.

[13] AFHYPAC (Association française pour l'hydrogène et les piles à combustible) Production et consommation d'hydrogène aujourd'hui. Mémento de l'hydrogène. Fiche 1.3., (n.d.). http://afhy-pac.org/documents/tout.savoir/Fiche_1.3_revision_fevrier_2008.pdf. (accessed June 7, 2018).

[14] K. Mazloomi, N.B. Sulaiman, H. Moayedi, Electrical efficiency of electrolytic hydrogen production, Int. J. Electrochem. Sci. 7 (2012) 3314–3326.

Alejandro Martínez Henríquez   Promotor: Vincent Lemort

[15]   C. Coutanceau, S. Baranton, T. Audichon, Hydrogen Electrochemical Production, in: Hydrog. Electrochem. Prod., Elsevier, London, 2018: pp. 1–6. doi:10.1016/B978-0-12-811250-2.00001-7.

[16]   Advantages and disadvantages of Solar Photovoltaic – Quick Pros and Cons of Solar PV - Renewable Energy World, (n.d.). https://www.renewableenergyworld.com/ugc/articles/2012/12/advantages-and-disadvantages-of-solar-photovoltaic--quick-pros-and-cons-of-solar-pv.html (accessed May 15, 2018).

[17]   S. Dubey, J.N. Sarvaiya, B. Seshadri, Temperature dependent photovoltaic (PV) efficiency and its effect on PV production in the world - A review, Energy Procedia. 33 (2013) 311–321. doi:10.1016/j.egypro.2013.05.072.

[18]   The Netherlands lags far behind European renewable energy goals, (n.d.). https://www.iamexpat.nl/expat-info/dutch-expat-news/netherlands-lags-far-behind-european-renewable-energy-goals (accessed May 15, 2018).

[19]   F.Z. Aouali, M. Becherif, A. Tabanjat, M. Emziane, K. Mohammedi, S. Krehi, A. Khellaf, Modelling and experimental analysis of a PEM electrolyser powered by a solar photovoltaic panel, Energy Procedia. 62 (2014) 714–722. doi:10.1016/j.egypro.2014.12.435.

[20]   O. Atlam, An experimental and modelling study of a photovoltaic/proton-exchange membrane electrolyser system, Int. J. Hydrogen Energy. 34 (2009) 6589–6595. doi:10.1016/j.ijhydene.2009.05.147.

[21]   P. Poggi, C. Darras, M. Muselli, G. Pigelet, The PV-hydrogen MYRTE platform - PV output power fluctuations smoothing, Energy Procedia. 57 (2014) 607–616. doi:10.1016/j.egypro.2014.10.215.

[22]   Energy Mix: Definition and Facts | Planète Énergies, (n.d.). https://www.planete-energies.com/en/medias/close/about-energy-mix (accessed May 15, 2018).

[23]   J. Larminie, A. Dicks, Fuel Cell Systems Explained, Wiley, Chichester, 2003. doi:10.1002/9781118878330.

[24]   N. Bizon, N. Mahdavi-Tabatabaei, F. Blaabjerg, E. Kurt, Energy Harvesting and Energy Efficiency, Springer, Cham, 2017. doi:10.1007/978-3-319-49875-1.

[25]   A. Brisse, J. Schefold, M. Zahid, High temperature water electrolysis in solid oxide cells, Int. J. Hydrogen Energy. 33 (2008) 5375–5382. doi:10.1016/j.ijhydene.2008.07.120.

[26]   K. Zeng, D. Zhang, Recent progress in alkaline water electrolysis for hydrogen production and applications, Prog. Energy Combust. Sci. 36 (2010) 307–326. doi:10.1016/j.pecs.2009.11.002.

[27]   F. Marangio, M. Santarelli, M. Calì, Theoretical model and experimental analysis of a high pressure PEM water electrolyser for hydrogen production, Int. J. Hydrogen Energy. 34 (2009) 1143–1158. doi:10.1016/j.ijhydene.2008.11.083.

[28]   B. Bensmann, R. Hanke-Rauschenbach, I.K. Peña Arias, K. Sundmacher, Energetic

Alejandro Martínez Henríquez   Promotor: Vincent Lemort

evaluation of high pressure PEM electrolyzer systems for intermediate storage of renewable energies, Electrochim. Acta. 110 (2013) 570–580. doi:10.1016/j.electacta.2013.05.102.

[29]   N. Job, Description of electrochemical cells, in: Electrochem. Energy Convers. Storage, University of Liege, Liege, 2018.

[30]   S.S. Makridis, Hydrogen storage and compression, in: R. Carriveau, S. Ting (Eds.), Methane Hydrog. Energy Storage, The Institution of Engineering and Technology, London, 2016: pp. 1–28. doi:10.1049/PBPO101E_ch1.

[31]   Hydro-Pac: high pressure gas compressors, pumps and related products, (n.d.). http://www.hydropac.com/how-intensifiers-work.html (accessed May 15, 2018).

[32]   P. Fischer, J. Schefer, K. Yvon, L. Schlapbach, T. Riesterer, Orthorhombic structure of γ-TiFeD≈2, J. Less Common Met. 129 (1987) 39–45. doi:10.1016/0022-5088(87)90031-2.

[33]   R.L. Berry, G. V. Raynor, IUCr, The crystal chemistry of the Laves phases, Acta Crystallogr. 6 (1953) 178–186. doi:10.1107/S0365110X53000557.

[34]   A. Léon, Hydrogen Technology. Mobile and Portable Applications, Springer, Berlin, 2008. doi:10.1017/CBO9781107415324.004.

[35]   R. Ströbel, M. Oszcipok, M. Fasil, B. Rohland, L. Jörissen, J. Garche, Journal of power sources., 2002. https://www.infona.pl/resource/bwmeta1.element.elsevier-9c4f5506-1acc-377d-a48d-e513a7f53d34 (accessed June 7, 2018).

[36]   P. Muthukumar, M.P. Maiya, S.S. Murthy, Experiments on a metal hydride based hydrogen compressor, Int. J. Hydrogen Energy. 30 (2005) 879–892. doi:10.1016/j.ijhydene.2004.09.003.

[37]   P. Dewallef, Renewable Energies, University of Liege, Liege, 2017.

[38]   O. Atlam, M. Kolhe, Equivalent electrical model for a proton exchange membrane (PEM) electrolyser, Energy Convers. Manag. 52 (2011) 2952–2957. doi:10.1016/j.enconman.2011.04.007.

[39]   I. EG&G Technical Services, Fuel Cell Handbook, U.S. Department of Energy, National Energy Technology Laboratory, Morgantown, 2002. doi:10.1002/zaac.200300050.

[40]   G. Monterey, Energy requirements for hydrogen gas compression and liquefaction as related to vehicle storage needs, 2009. http://www.hydrogen.energy.gov/storage.html.

[41]   R. Luthander, J. Widén, D. Nilsson, J. Palm, Photovoltaic self-consumption in buildings: A review, Appl. Energy. 142 (2015) 80–94. doi:10.1016/j.apenergy.2014.12.028.

[42]   N. Job, Electrochemical energy conversion and storage, University of Liege, Liege, 2018.

Alejandro Martínez Henríquez   Promotor: Vincent Lemort

[43]   M. Santarelli, S. Macagno, A thermoeconomic analysis of a PV-hydrogen system feeding the energy requests of a residential building in an isolated valley of the Alps, Energy Convers. Manag. 45 (2004) 427–451. doi:10.1016/S0196-8904(03)00156-0.

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