Bachelorthesis

Model of a hybrid system powered by renewable energies in MATLAB/Simulink

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Statutory declaration

Hereby I assure, Tarmo Tukiainen, that I have written the present work "Model of a hybrid system powered by renewable energies in MATLAB/Simulink" independently and have used no sources and aids other than those indicated in the bibliography.

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Name Datum

Abstract

This paper describes the functionality of hybrid energy system (HES) located near Stuttgart, Germany. The hybrid system consists of photovoltaics, a battery bank, an electrolyser and a hydrogen storage tank. The hydrogen is meant to be sold for use in hydrogen busses belonging to the local public transport. This paper aims to build a MATLAB model for the Institute of Sustainable Energy Engineering and Mobility (INEM) which they can use in their later projects. The purpose is a calculation of the system and to see how the battery system, electrolyser and storage system should be sized for optimum performance, with regards to an adequate hydrogen production amount. This paper also gives a short analysis whether it would be better to have the FCV fuelling station on- or off-site.

Kurzfassung

Die vorliegende Arbeit beschreibt die Funktionalität von einem Hybrid-Energie-System (HES) in der Nähe von Stuttgart, Deutschland. Dieses HES besteht aus einer PV-Anlage, eine Batterie, ein Elektrolyseur und ein Wasserstofftank. Der Wasserstoff wird verkauft für die Wasserstoffbusse in die lokal öffentlicher Verkehr. Dieses Papier soll bauen ein MATLAB modell für die Institut für Nachhaltige Energietechnik und Mobilität (INEM), damit sie es in späteren projekten verwenden können. Das Modell soll dabei helfen, die richtige Größen verschiedener Kompotenten im HES zu bestimmen, damit eine angemessene Menge Wasserstoff erzeugt und eine hohe Nutzungsrate erreicht wird. Diese Arbeit analysiert zusätzlich ob es besser ist die FCV-Tankstelle on-site oder off-site zu betreiben.

Contents

Abbreviations

Abbreviation	**Description**
2DS	2°C Scenario
CO_2	Carbon dioxide
FCV	Fuel cell vehicle
FPR	Fiber Reinforced Polymer
HES	Hybrid Energy System
INEM	Institut für Nachhaltige Energietechnik und Mobilität
IPCC	Intergovernmental Panel on Climate Change
NPR	Nominal Production Rate
RE	Renewable energy
PV	Photovoltaic
PEM	Polymer Electrolyte Membrane
PEME	Polymer Electrolyte Membrane Electrolysis
PCpV	Power Consumption per Volume (of H_2 gas produced)
HFCV	Hydrogen fuel cell vehicle

1. Introduction

1.1. Motivation

Exploitation of fossil fuels in energy production and transport has allowed humanity to progress technologically at a rate never seen before in history. But because the realization of the problems caused by this free exploitation, societies are now trying to find fossil-free alternatives. So, combatting problems such as climate change means a complete revamp of our energy production and transport sectors into something sustainable.

Renewable energy (RE) sources such as wind power and solar power via photovoltaic (PV) panels have widely been accepted as the two main alternatives in energy production. But because of the short-term and seasonal fluctuating nature of these energy sources, there is a need to find a way to properly store this energy.
Battery technology is the leading candidate at the moment, yet it is not necessarily the best one due to the fact that chemical batteries lose 1-5% of their energy content in one hour and so are only suitable for short-term storage [1].

Acting fast is required to achieve the emission reductions agreed upon in the Paris climate agreement and to keep the warming within the 2DS. In the EU this means reducing the Unions CO_2 emissions from 3 500 Mt of CO_2 today to 770 Mt of CO_2 in 2050. Hydrogen has the potential to supply up to a quarter of the EUs energy demand in 2050, equal to 2 250 TWh worth of H_2. In comparison, heating 52 million households requires approximately 465 TWh [2].

Due to this reason alternative energy storage methods are being researched continuously. A popular candidate is hydrogen, an energy carrier, which does not lose its energy content over time and can be utilized in various uses via a fuel cell. In this study electricity produced by PV panels is used in polymer electrolyte membrane-, sometimes called proton exchange membrane (PEM) electrolysis to produce hydrogen. A MATLAB tool is developed to compare different scenarios and sizing methods of the components.

1.2. Chapter overview

Chapter one describes the motivation behind this work. Chapter two goes through the theory involved in the technologies that are the focus of this study. Chapter three focuses on the work in MATLAB and the formulas and methods used. In chapter 4 the MATLAB program is tested, different scenarios compared and the optimum one is chosen. Chapter 5 offers an overview and a summary of the results and findings. In chapter 6 all the sources used in this work are listed.

2. Basics and state of the art

The purpose of this chapter is to analyse the basic principles behind the technology relevant to this work. The chapter has been divided into four parts. First in subchapters 2.1 and 2.2 this paper focuses on solar energy, PVs and battery technology. Next in subchapter 2.3 the paper explains the relevant information about hydrogen and electrolysis. Lastly in subchapter 2.4. hydrogen storage and compression are discussed.

2.1. Solar energy and photovoltaics

Hydrogen plays an important role when it comes to solar energy, considering that 75% of the Sun is formed by hydrogen (23% He and 2% heavy elements). The Sun gets its energy from its inner nuclear reactions where four hydrogen nuclei form into a helium nucleus in nuclear fusion. Every second $6 \cdot 10^{11}$ kilograms of hydrogen is transformed into helium and some of this mass is transformed into energy according to Einstein's law of $E = mc^2$, thus giving off the energy as electromagnetic radiation [3].

The amount of Suns radiation that arrives on Earth is enormous and in theory is enough to cover humanity's energy need ten thousand fold. About one third of the received radiation is reflected to space, but the amount received by surface is still as massive as $3{,}9 \cdot 10^{24}$ MJ per year [4].

The quantity of solar energy that reaches Earth outside the planet's atmosphere is called the solar constant and it is 1367 W/m^2 [3]. The solar constant is measured on a surface perpendicular to the rays. After the scattering and diffusing caused by the atmosphere the utilizable amount on the surface, in Germany, is usually between 900-1200 kWh/m^2, as shown in Figure 1.

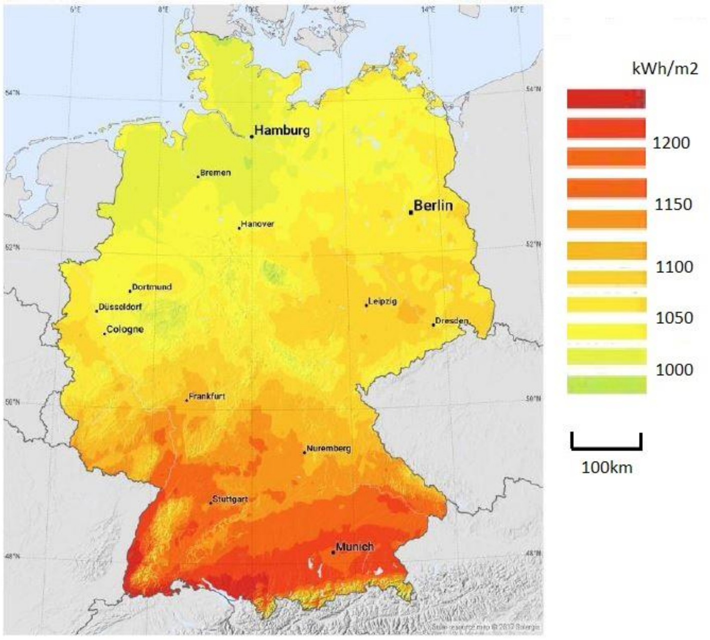

Figure 1. Solar irradiation in Germany, kWh/m2 (edited from [5])

To utilize this energy, we use photovoltaic (PV) cells designed to convert the sunlight into electrical energy. These cells are connected in chains to form panels which in turn can be combined to form solar arrays [6]. Because of this scaling possibility, PV panels can answer an energy need of virtually any size. The price of implementing PV technology in a sensible scale has also reached maturity and is starting to be very competitive with traditional energy production methods, partly depending on where you are geographically located. In Germany, the electricity generation costs of decentralized PV systems are less than 10 cents/kWh [7].

The operating principle of PVs is relatively simple. Each PV cell has a positive and a negative layer (p-n junction) which between them create an electric field. Photons from the Sun upon arrival to Earth hit the layers in the cell and are absorbed by the semiconductor material, freeing electrons. These charge carrier pairs are then separated in the electric field of the p-n junction. This electric current is then harnessed by cables connected to the two sides, positive and negative, of the cell [7, 8].

There are many different materials that can be used as the semiconductor material. The electrical conductivity of semiconductors is almost zero in absolute zero temperature and increases with rising temperature. In approximately 90% of all panels today, silicon is the semiconductor material and as seen in figure 2, its advantages include a very good conductivity scale. It is also the second most abundant material on Earth, and it offers a combination of low cost, high efficiency, and a long lifetime.

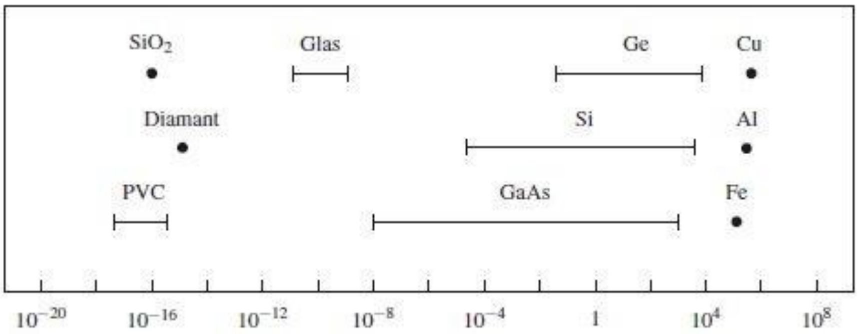

Figure 2. Electrical conductivity σ of different materials (Ωcm)-1 [7]

2.2. Battery technology

The rise of portable electronics from Walkman cassette players to the latest smartphones created the demand to store energy so it can be used anywhere. This demand was met with batteries that have seen rapid development over the years after first being introduced in the early 1800s. The “modern” rechargeable battery can be considered to have begun in 1859 when a French scientist, Gaston Planté, produced the first lead-acid rechargeable battery [9].

Right now, the most prominent battery technology is the lithium-ion battery which can be used in a wide range of appliances partly thanks to its high volumetric and gravimetric energy density when compared with other battery types, as demonstrated in figure 3. Lithium-ion batteries are a popular choice because of their long cycling life and high energy capacity [10].

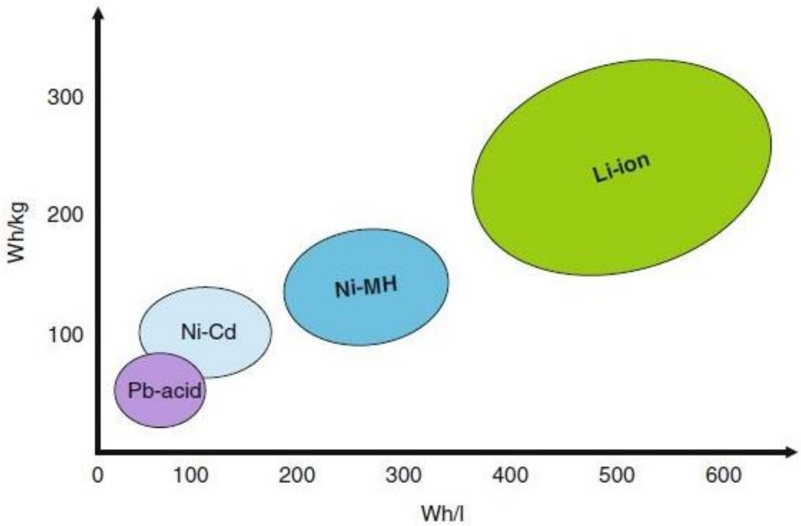

Figure 3. Volumetric- (Wh/l) and gravimetric (Wh/kg) energy density for different battery types [11]

The working principle of Li-ion cells can be understood as a “rocking-chair” principle, proposed by M.S. Whittingham in the 1970s, because within the cell the lithium ions swing between the anode and the cathode through an organic liquid electrolyte, in a similar manner as a rocking chair swings from side to side [11].

The anode is usually made of hard carbon, graphitic carbon or treated graphite while the cathode consists of a layered oxide, spinel (i.e. lithium manganese oxide) or a polyanion (i.e. lithium iron phosphate). The electrolyte can be generalized to contain lithium-containing salt dissolved in a solvent that contains a mixture of organic carbonates [11].

All Li-ion batteries have a certain cycle life, the amount of charges and discharges they can withstand, given by the manufacturer. But these lifetimes are not always as in the given datasheets. Lithium-ion cells can degrade can also be affected by temperature, operation of extended voltage levels state of charge and depth of discharge [12].

2.3. Hydrogen and electrolysis

2.3.1. Hydrogen

Hydrogen (H_2) is the most abundant element in the universe yet it cannot be found in its pure molecular form on Earth. The most common isotope of hydrogen consists of one proton and one electron.

Hydrogens is in solid form at 11 Kelvins (-262°C) and stays liquid only in a small zone before turning into gas in its boiling point at 20,3 Kelvins, above which it is always in gaseous form in normal atmospheric pressure, as illustrated by figure 4. It has a very wide ignition range, the mixture being able to ignite from a hydrogen concentration of 4 vol% to 77 vol%. But despite its wide flammability range, hydrogen vehicles use fuel cells instead of combustion engines [13].

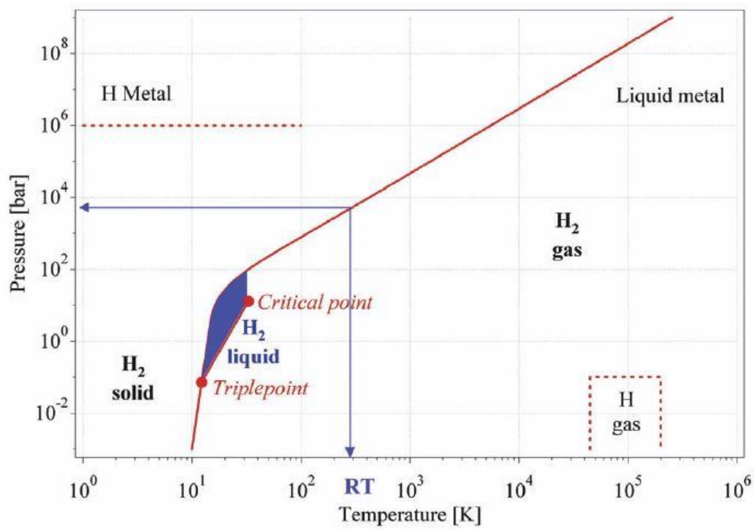

Figure 4. Phase diagram of hydrogen [14]

There is also collaboration between SSAB, LKAB and Vattenfall to replace coking coal, used in ore-based steel making, with fossil free hydrogen by 2045. This could eventually eliminate virtually all CO_2 emissions associated with steel making (currently ~7% of global CO_2 emissions). Though eliminating the emissions completely would require a massive increase in clean electricity production [15].

There are numerous ways to produce hydrogen but as seen in Figure 5, the greenhouse gas emissions of producing hydrogen with reforming methods are much higher than those of renewable electricity electrolysis. Therefore, using steam reforming in the long term is not feasible when you consider that the reason to start using hydrogen in the first place is to cut down emissions in the energy sector. Producing hydrogen with surplus energy from renewable sources guarantees the lowest emissions and with electrolysis you get the high purity hydrogen demanded by many end-uses [13, 14].

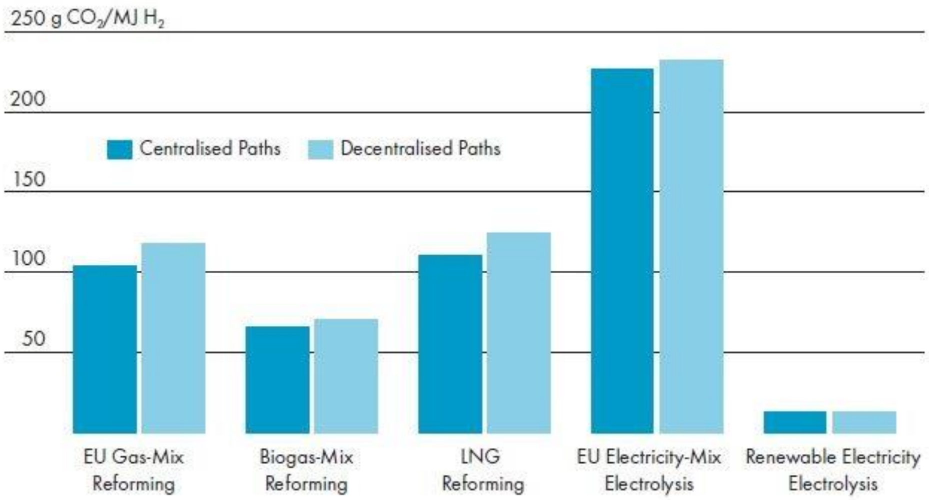

Figure 5. GHG emissions of different hydrogen supplies (in CO_2 eq./MJ H_2) [13]

2.3.2. Electrolysis

Electrolysis uses electricity to split water molecules into hydrogen and oxygen. An electrolyser consists of an DC electricity source and two noble-metal-coated electrodes, the negative electrode is called an anode and the positive one is cathode, that are separated by an aqueous solution called the electrolyte. An electrolyser consists of separate cells and by combining these, the electrolysers hydrogen production can be tailored to different requirements just like with PV cells.

Different types of electrolysis techniques exist such as alkaline-, polymer electrolyte-, anion exchange membrane- and solid oxide electrolysis. Typical water electrolysers reach an efficiency of 60-80%. The price of producing hydrogen via electrolysis is tightly tied with the price of electricity, which is also why electrolysis still plays such a small role (about 5%) of global hydrogen production. For widespread introduction of the hydrogen-economy it is vital to use surplus energy from RE sources for electrolysis [13].

In this project a PEM electrolyser is chosen due to its lower cost of operation and ability to function with a wide power input range [16].

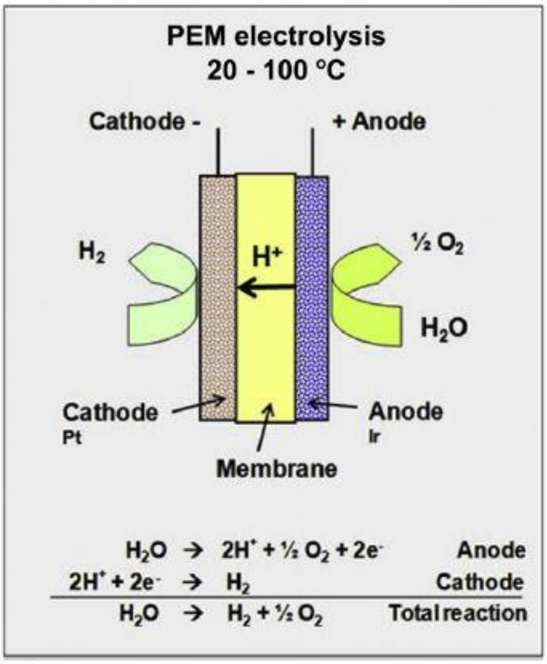

Figure 6. Working principle of PEM electrolysis [17].

As shown in Figure 6, in a PEM electrolyser the cathode and anode are bonded together forming the membrane electrode assembly (MEA) and a polymer membrane is the electric conductor. Water molecules are supplied to the anode where they break down to form oxygen, protons and electrons (Eq. 1.1). The protons move through the conductive membrane to the cathode where they, together with the electrons, re-combine with the result being hydrogen gas (Eq. 1.2) [17].

Anode: $H_2O \rightarrow 2H^+ + \frac{1}{2}O_2 + 2e^-$ (Eq. 1.1)

Cathode: $2H^+ + 2e^- \rightarrow H_2$ (Eq. 1.2)

Overall: $H_2O \rightarrow H_2 + \frac{1}{2}O_2$ (Eq. 1.3)

The PEM electrolysis (PEME) has some advantages over other means of electrolysis, mostly because the nature of the membrane itself. The PEM provides high proton conductivity and allows for compact system design together with high pressure operation, partly because of its low thickness (~20-300µm). They can achieve a current density of up to 2 A cm^{-2} thus reducing costs of operation. Because the gas crossover rate of the PEM is low, the electrolyser can work with a wide power input range [16].

One potentially negative aspect of PEME is that the catalyst material on the anode is iridium which is one of the rarest metals on earth. This is the chosen material because the anode and cathode both must be coated with a corrosion resistant material in the PEME. Iridium’s demand has risen due to its usage in home electronics and its price may further rise if PEME technology becomes the leading choice for electrolysis [16].

2.4. Hydrogen compression and storage

There are multiple ways to store hydrogen as an energy medium, some techniques are more widely used whereas others are still in their infancy while being intensively researched. These methods include physical storage as a compressed hydrogen gas (CGH_2) or as liquid hydrogen (LH_2) and materials-based storage, sometimes called solid storage of hydrogen (SSH_2). Of these, the first two are more widely in industrial use and fuel cells and fuel cell vehicles rely on gaseous hydrogen storage.

Materials-based storage is researched extensively and may come a competitive alterative in the future, particularly due to improved safety and volumetric energy density achieved by these technologies. Materials-based storage still has many problems to overcome such as those related to thermal management and up-scaling [16].

Liquid hydrogen, though an effective storage method, also has some disadvantages. These include the required energy input to liquefy the gas and the strict criteria that container technology must meet to achieve temperature and pressure stability. One weak link, with the biggest risk for leaking, is the point between the two cryogenic storages. For example, the point between storage tank and vehicle, called “cryogenic coupling”. But in recent years progress has been made also in this sector [18].

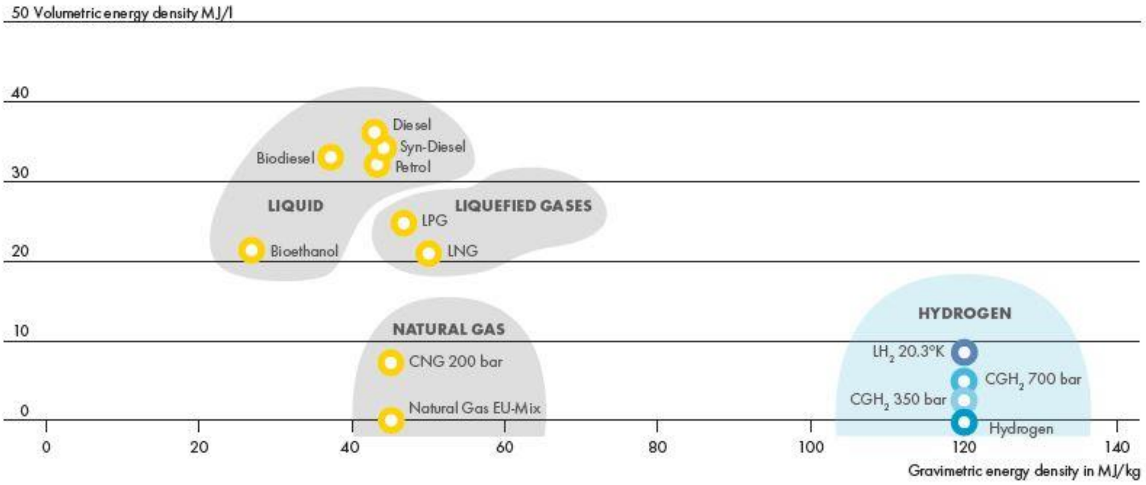

Figure 7. Energy densities of different fuels [13].

As can be seen from Figure 7, the volumetric energy density of H_2 in ambient conditions is just 0,01 MJ/l and hence the density must be significantly increased before storage. CGH_2 is the most popular storage method especially in the mobility sector. Gaseous hydrogen is stored in high-pressure cylinders where the industry standard pressure is usually at 350 bar or 700 bar. The storage tank material should have a very high tensile strength, low density and it should not react with hydrogen or allow H_2 to diffuse into it.

Common choice of materials includes austenitic stainless steels such as AISI 316 and -304, aluminium alloys and carbon fibre materials. There also exists large-scale underground storage facilities for gaseous hydrogen, such as salt cavities, which benefit from lower investment- and construction costs, low leakage rates and minimal risk of hydrogen contamination. The same kind of pipeline storage that exists for natural gas has also been suggested for hydrogen and it is estimated that 12 tonnes of hydrogen could be stored per kilometre of pipeline. [14, 19].

	Pressure [bar]			
T (°C)	**1**	**10**	**30**	**300**
0	0,0887	0,8822	2,6630	22,1510
25	0,0813	0,8085	2,4400	20,5370
50	0,0750	0,7461	2,2510	19,1490
80	0,0687	0,6865	2,0596	16,9080

Table 1. Hydrogen gas density in different pressures in kg/m^3

When hydrogen gas is compressed to 350 bar or 700 bar its volumetric energy density increases to 2,9 MJ/l and 4,8 MJ/l respectively. From the data in Table 1 it is apparent that the gas temperature should be as low as possible to guarantee optimum density and that maximum compression pressure should be targeted.

Usually the ideal gas law (PV = nRT) predicts the behaviour of gasses in different environments. But this is not the case with hydrogen due to the nature of hydrogen gas: the hydrogen molecule is highly polarised and thus the attraction forces between molecules change the gas pressure slightly [18].
This results in that hydrogen gas always occupies more space than the ideal gas law predicts. Different equations have been proposed for real gases to predict their behaviour, such as the inclusion of a compressibility factor, Z. Compressibility factor is added to the ideal gas law in the following way:

$$PV = nZRT \qquad \text{(Eq. 2.1)}$$

It is worth noting that in low pressures the compressibility factor Z equals one and can be neglected [20].

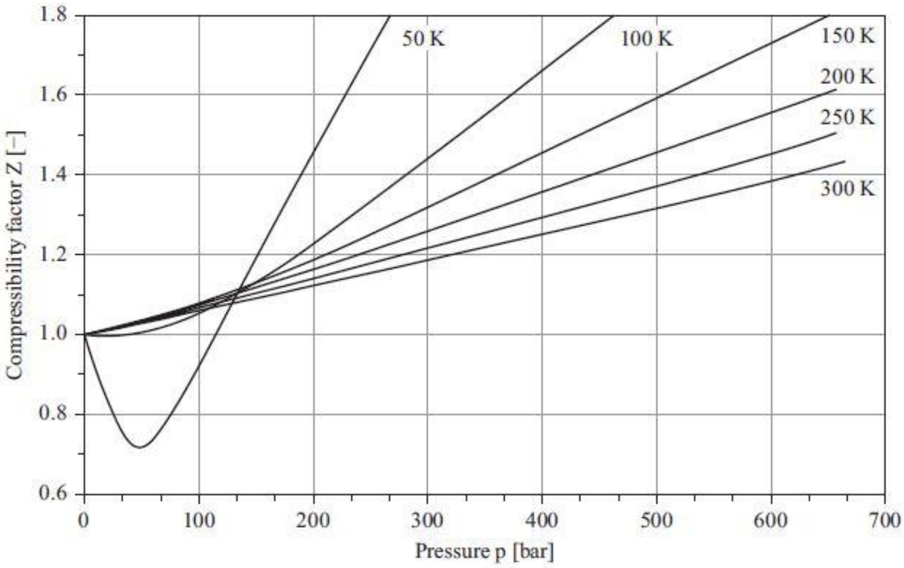

Figure 8. Compressibility factor Z of H_2 in different temperatures [20]

Figure 8 illustrates that to compress hydrogen to 300 bars in ambient temperature would give us a compressibility factor of 1,2. This means that to compress a given volume of hydrogen gas you would need the energy to compress 1,2 times that amount. Another equation proposed to assist in real gas calculations is the 'van der Waals' model [18], where constants α and b are experimentally determined:

$$\left(P + n^2 * \frac{\alpha}{V^2}\right) * \left(\frac{V}{n} - b\right) = RT \qquad \text{(Eq. 2.2)}$$

Because the compression of hydrogen is a polytropic process the temperature of the gas changes during compression thus increasing the final temperature. Cooling during the compression process could reduce the work required. But obtaining continuous cooling throughout the entire process is difficult and would require complicated cooling systems to guarantee uniform removal of heat and a uniform temperature distribution in the gas. A better way to do this is to use a multistage compressor and cooling the gas between compressor stages using an intercooler [18].

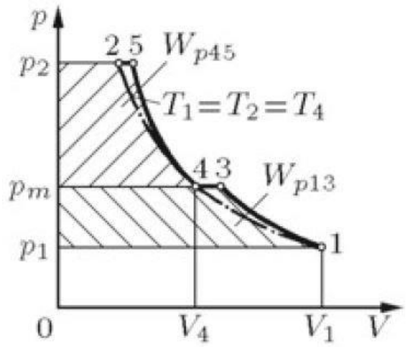

Figure 9. Visualization of the compression process [21]

To achieve minimum work in multistage compression, the pressure ratio should be identical in both stages as illustrated by figure 9. The optimal intermediate pressure, P_m, can then be found with (Eq. 2.3)

$$P_m = \sqrt{P_1 * P_2} \qquad \text{(Eq. 2.3)}$$

2.5. Overview of the system

The system that this work is meant to analyse consist of PV panels, a PEM electrolyser, a battery, a hydrogen storage tank and compressors. The energy from the PV panels is used to create hydrogen with one or two electrolysers. This hydrogen is then compressed to 300 bar. It can be compressed further up to pressures of 800 or 1000 bar if necessary.

3. MATLAB Files

The intention of this chapter is to describe the MATLAB files associated with this work and to explain how they are used. The files are demonstrated in the order they are to be executed once the experiment is run. Figure 10 illustrates the MATLAB files and shows the Excel files that are automatically created, summarizing the resulting data.

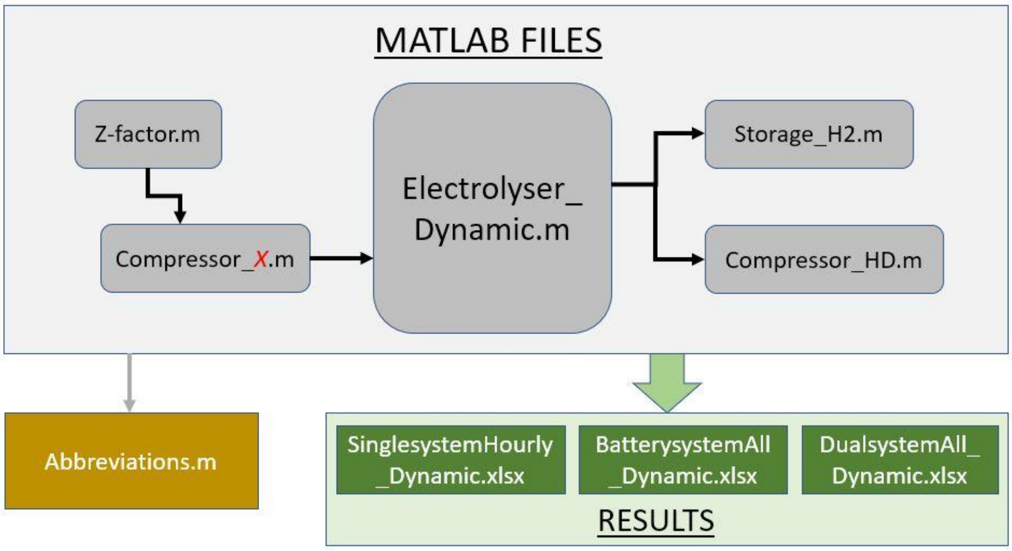

Figure 10. Illustration of the MATLAB files and the resulting Excel files

3.1. Compressibility factor

As section 2.4 explains, hydrogen does not behave like an ideal gas under high pressures and that multiple predictions have been made as demonstrated by [18, 20]. This part helps to predict hydrogens behaviour in different environments.

By using formulas provided by [22] and [21] we can determine the compressibility factor, Z. Section 3.1.1. is meant if you only need to calculate a single Z-factor, for example when you use a one-stage compressor. Section 3.1.2. describes the main file meant for two-stage compression.

3.1.1. Single-stage Z-factor

This file (*Z_factor_1stage.m*) enables the user to quickly calculate a single compressibility factor in case a single-stage compressor is used in one point of the process.

The compressibility factor is calculated with these steps by combining the Van der Waals equation and the virial equation of state according to Babel [22].

$$0 = V_{mz}^3 - \left(b + \frac{RT}{p}\right) * V_{mz}^2 + \left(\frac{a}{p}\right) * V_{mz} - \frac{ap}{b} \quad \text{(Eq. 3.1)}$$

$$V_m = \frac{RT}{p} \quad \text{(Eq. 3.2)}$$

$$Z = \frac{V_{mz}}{V_m} \quad \text{(Eq. 3.3)}$$

Where *a* and *b* are Van der Waals constants, 24645,79 $Nm^4/kmol^2$ and 0,0267 $m^3/kmol$ respectively, *R* is the universal gas constant, *T* is the compression temperature in Kelvins and *p* is the compression pressure in Pascals.

Only input variables required in this step are the gas temperature in Kelvins and the gas pressure in Pascals. Once these values are inserted and the file is executed, the resulting compressibility factor will show in the workspace as Z.

3.1.2. Two-stage Z-factor

As demonstrated in the end of section 2.4. multistage compression should be used to guarantee minimum work in the compression process. When compressing in two stages, this file (*Z_factor.m*) is used.

The input variables in this file are:

T	Gas temperature [K]	(Var 1.1)
P1	Gas inlet pressure [Pa]	(Var 1.2)
P2	Gas outlet pressure [Pa]	(Var 1.3)
Pm	Gas int.med. pressure [Pa]	(Var 1.4)

Compressibility factor is calculated according to (Eq. 3.1), (3.2) and (3.3). Once the above mentioned input variables are decided and inserted into the file, execute the file. This will result in three different compressibility factors: Z-factor in inlet pressure (*Z1*), Z-factor in outlet pressure (*Z2*) and Z-factor in intermediate pressure (*Zm*). These values are then later used in *'Compressor_2-stage.m'*. An important trend of the Z-factor is its relation to both pressure and temperature, as indicated in Table 2.

	Pressure [bar]			
T (°C)	**30**	**100**	**300**	**700**
0	1,0210	1,0780	1,2712	1,7215
25	1,0208	1,0741	1,2518	1,6616
50	1,0200	1,0704	1,2352	1,6113
80	1,0190	1,0664	1,2181	1,5606

Table 2. Hydrogen compressibility factor in different temperature and pressure.

3.2. Compression

3.2.1. Single-stage compression

When dealing with low pressures, or for some other reason single-stage compression is chosen, this file (*Compressor_1stage.m*) calculates the work needed to compress one cubic meter of gas according to [21]. To calculate the compressibility factor for this step, refer to section 3.1.1.

The required input variables for this file are:

T	Temperature [°C]	(Var 2.1)
P1	Inlet pressure [Pa]	(Var 2.2)
P2	Outlet pressure [Pa]	(Var 2.3)
CEff	Compressor electrical efficiency	(Var 2.4)

To calculate the necessary work, we begin by first calculating the volume occupied by one Nm^3 (V_N) of hydrogen gas in inlet pressure P1 (V_1).

$$V_1 = \left(\frac{P_{atm}}{P_1}\right)^{\frac{1}{k}} * V_N \qquad \text{(Eq. 3.4)}$$

The work required to compress this volume of hydrogen gas into outlet pressure *P2* is then calculated [21] and multiplied by the compression factor *Z*.

$$W = \frac{k * P_1 * V_1}{k-1} * \left(\left(\frac{P_2}{P_1}\right)^{\left(\frac{k-1}{k}\right)} - 1\right) * Z \qquad \text{(Eq. 3.5)}$$

Result from this calculation is expressed in Newton meters and to convert it to kilowatt hours the following conversion is done.

$$W_{kWh} = W * 2{,}777778 * 10^{-7} \quad \text{(Eq. 3.6)}$$

Ratio of specific heats is interpolated from the values illustrated in Table 3.

T (°C)	Gas	*k*
-181	H_2	1,597
-76		1,453
20		1,41
100		1,404
400		1,387
1000		1,358
2000		1,318

Table 3. k-values for hydrogen in different temperatures (based on [23])

3.2.2. Two-stage compression

As instructed in section 3.1.2 you should now have three compressibility factors in your MATLAB workspace for this file (*Compression_2stage.m*). Z_1 for inlet pressure, Z_m optimum intermediate pressure and Z_2 for outlet pressure.

This file requires the following input variables:

CEff	Compressor efficiency	(Var 2.5)
T	Temperature [°C]	(Var 2.6)
Z1	Z-factor for Pressure P_1	(Var 2.7)
Zm	Z-factor for pressure P_m	(Var 2.8)
Z2	Z-factor for pressure P_2	(Var 2.9)
P1	Inlet pressure [Pa]	(Var 2.10)
P2	Outlet pressure [Pa]	(Var 2.11)

Just like in section 3.2.1. the *k*-value is interpolated from Table 3 and volume of one Nm^3 is calculated according to (Eq. 3.4). Next the same is repeated to calculate what is the volume for this amount of hydrogen in intermediate pressure P_m, this will be denoted as V_2.

The process to calculate the volume requires three steps which are explained below.

Firstly (Eq. 3.4) is repeated to get V_1. After that the density of the gas in given pressure, P_1, is calculated with the mass and number of moles in that given volume. Density is calculated according to Zhengs method [24].

$$DensP_1 = \frac{P_1 * M}{R * Z_1 * T} \quad \text{(Eq. 3.7)}$$

$$m = \frac{V_1}{DensP_1} \quad \text{(Eq. 3.8)}$$

$$n = \frac{(m * 1000)}{M} \quad \text{(Eq. 3.9)}$$

Where *R* is the universal gas constant, *T* is the temperature in Kelvins, *m* equals mass in kilograms, *M* is the molecular weight of hydrogen in grams and *n* is the number of moles in the given amount of gas. After having acquired this information we can calculate the volume of hydrogen in pressure P_m according to Makridis [20].

$$V_2 = \frac{n * Z_m * R * T}{P_m} \quad \text{(Eq. 3.10)}$$

We then calculate the work required for the compression according to [21]. Some sources have calculated this slightly differently. Whereas some books, like [21], use volume as a variable, Tzimas [18] replaces this variable with temperature. This paper uses the former, due to uncertainties about the consistency of gas temperature during compression.

$$W = \frac{k * P_1 * V_1}{k - 1} * \left(\left(\frac{P_m}{P_1} \right)^{\frac{k-1}{k}} - 1 \right) * Z_m + \frac{k * P_m * V_2}{k - 1} * \left(\left(\frac{P_2}{P_m} \right)^{\frac{k-1}{k}} - 1 \right) * Z_2 \quad \text{(Eq. 3.11)}$$

$$W_{kWh} = W * 2{,}777778 * 10^{-7} \quad \text{(Eq. 3.12)}$$

Finally, the resulting compression work is converted from Newton meters per m^3 to kWh/m^3 in equation 3.12.

3.2.3. HD compressor

This file (*Compressor_HD.m*) is meant to get an overlook of the compressor work if the compression process is continued to an additional high-pressure storage which is usually around 800 to 1000 bars. It calculates the compressibility factor and compressor work per cubic meter according to sections 3.1.2. and 3.2.2. According to Tzimas [18], significantly less energy is required to compress hydrogen from 350 bar to 700 bar, than from ambient pressure to 350 bar and the result should reflect this.

3.3. Electrolysis

After executing the previous calculations next is the file (*Electrolyser_Dynamic.mlx*) for the whole electrolysis process. The objective of this file is to help analyse and determine the optimum sizing of the components. In order to do so we need to get outputs such as the hydrogen production amounts, utilization rates and how much of the incoming energy is left unspent.

The calculations are done for two different scenarios; one where the system consists of a single electrolyser and a battery, and one where the system consists of two electrolysers with no battery. For clarity the former scenario is from now on described as 'battery system', and the latter scenario is described as a 'dual system'.

This file is divided into segments, where in parts I-IV the preliminary solar data is organized into better readable forms, and in parts 1-12 the results are gathered. All abbreviations mentioned and not mentioned in this paper can be found in the MATLAB file called '*Abbreviations_Dynamic.m'*.

The efficiency of an electrolyser changes in accordance with the amount of hydrogen it is producing at each moment, as illustrated in figure 10. The efficiency parameters are different for every electrolyser and these parameters "are part of a manufacturer's know-how and consequently are not frequently disclosed" [25]. This paper utilizes the efficiency curve of a Siemens SILYZER 200 PEM electrolyser, but as said, the results are not 100 % applicable to other electrolysers. The results should still give the best available outlook on the sizing of components.

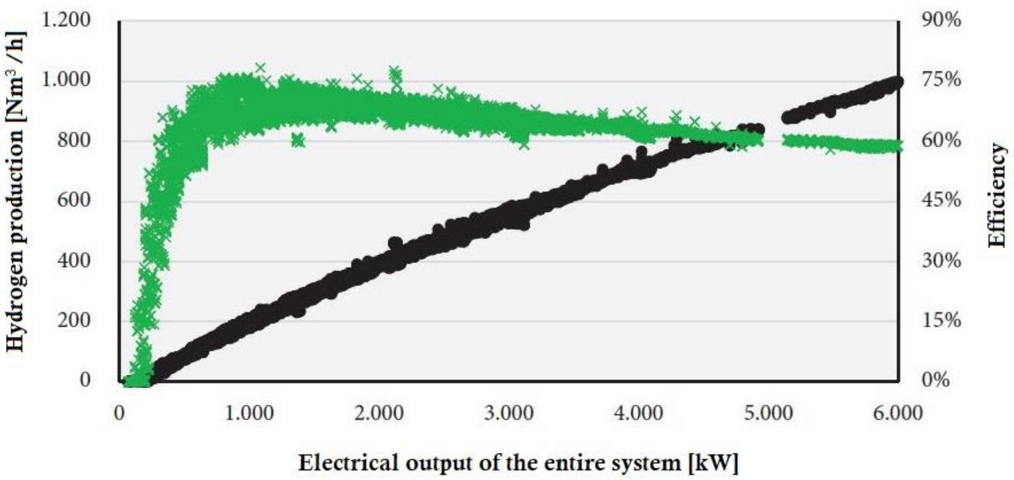

Figure 11. A typical production characteristic and efficiency curve of an example system (edited from [26])

3.3.1. Parts I-IV: Arranging the PV data

The excel file with data of the PV production for one year works as the basis for this MATLAB file. It contains the yearly output of the selected amount of PV panels for one year, with fifteen (15) minute intervals. This data is brought to MATLAB and converted from watt hours to kilowatt hours in part I. In file parts II and III the program combines the PV output into values corresponding intervals of one hour and one day.

3.3.2. Part 1: Input variables

In this part the input variables of different components are determined and after this no further action is required from the user. The required input variables are:

Npr	Nominal production rate [Nm^3/h]	(Var 2.12)
NMP	Nominal power [kW]	(Var 2.13)
PCpV	Power consumption [kWh/Nm^3]	(Var 2.14)
TempE	Operating temperature [°C]	(Var 2.15)
BtCap	Available battery capacity [kWh]	(Var 2.16)
Npr2	Nominal production rate [Nm^3/h]	(Var 2.17)
NMP2	Nominal power [kW]	(Var 2.18)
PCpV2	Power consumption [kWh/Nm^3]	(Var 2.19)
HVL	Hydrogen valve losses [%]	(Var 2.20)
BGL	Battery general losses [%]	(Var 2.21)
TankCap	Transport/storage capacity [kg]	(Var 2.22)

Nominal production rate, nominal power and power consumption depend on the electrolyser model and can be found in the data sheets provided by the manufacturer. It is important to notice that *Npr2*, *NMP2* and *PCpV2* indicate the values of the second electrolyser of the system. In case the user wants to ignore the possibility of a second electrolyser, these values should be set to zero.

It is important to notice that *BtCap* refers to the available capacity that the system can charge and discharge completely. It should thus be set to a smaller value than what is the actual battery size. With a depth of discharge of more than 50 % the battery life can decrease to under 1000 cycles, as shown in figure 12.

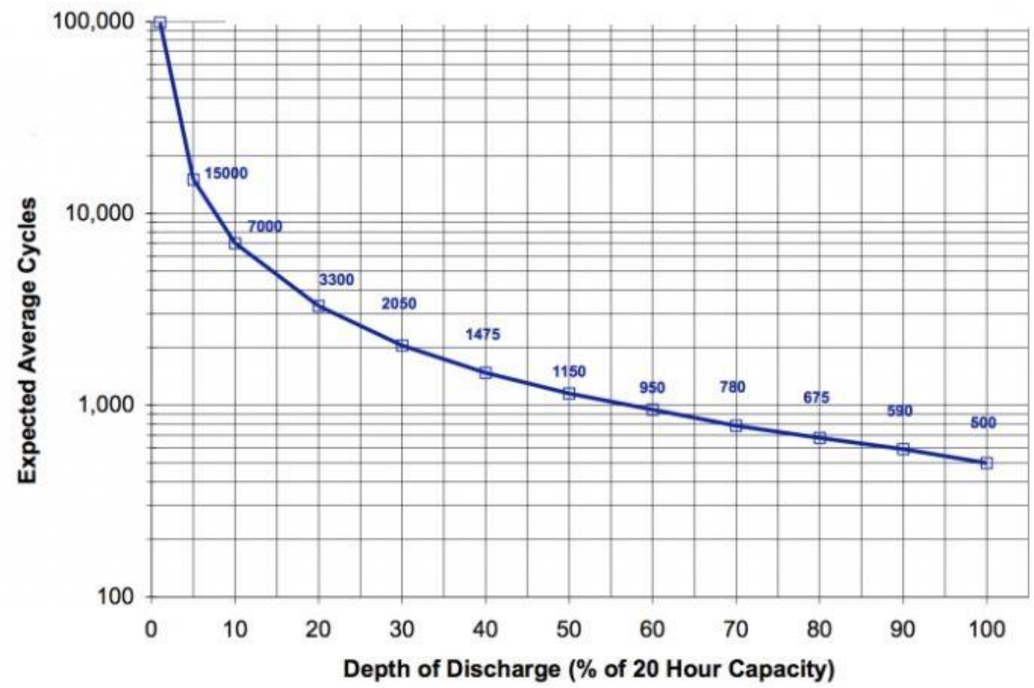

Figure 12. Expected average cycles vs. battery depth of discharge [27]

TankCap is meant for later analysing when estimating the location of the hydrogen filling station. With *TankCap* we can set a certain limit to the storage tank size and see on which time intervals it is filled. Most common tube trailers can carry a load of 500 kilograms of hydrogen, with container trailers reaching a maximum load of 1000 kilograms [13]. If the hydrogen filling station is located off-site, with *TankCap* we can estimate the frequency of transport needed. Or we can in general see how fast the local storage tank is filled.

For finding out later how many kilograms of hydrogen is produced, the density is calculated according to the input values inserted by the user. In low pressures the compressibility factor is almost equal to one, and can thus be neglected [20].

$$DensElec = \frac{P * M}{R * T} \qquad \text{(Eq. 3.13)}$$

Where *P* equals electrolysis pressure (Pa), *M* the molecular weight of hydrogen (2,0158 g/mol), *R* the universal gas constant and *T* the electrolysis temperature (Kelvin). Density is then given in kilograms per cubic meter.

3.3.3. Part 2: Hydrogen production of main electrolyser

The hydrogen production of the system depends on the efficiency of the electrolyser. In this paper, in absence of real-life parameters, the parameters of a Siemens SILYZER 200 electrolyser are used to estimate the efficiencies of different electrolysers. The hydrogen production amount is calculated according to an equation provided by Kopp [26].

$$H_2\, production = -6{,}45 * 10^6 * (P_{el})^2 + 0{,}2065 * P_{el} - 7{,}6559 \qquad \text{(Eq. 3.14)}$$

Where P_{el} is the energy the electrolyser uses to produce hydrogen. The production must cover at least 10 % of the nominal production rate of the electrolyser, otherwise the production is zero.

The following outputs are calculated in this part. The program also shows how many days of the year the electrolyser does not run on its own and shows this as *DNR1*. All of them are production rates from the primary electrolyser:

H2PVs_hourly	Hourly H_2 production data [m^3/h]	(Var 2.23)
H2PVs_daily	Daily H_2 production data [m^3/day]	(Var 2.24)
H2yr_kg_PVs	Hourly H_2 production data [kg/h]	(Var 2.25)
H2yr_kg_PVsdaily	Daily H_2 production data [kg/day]	(Var 2.26)
H2PV_Nm_sum	Total H_2 produced with 1^{st} electrolyser [m^3]	(Var 2.27)
H2PV_kg_sum	Total H_2 produced with 1^{st} electrolyser [kg]	(Var 2.28)
Efficiency_Ely	Efficiency of electrolyser at any moment	(Var 2.29)

3.3.4. Part 3-4: Power consumption

After determining the hydrogen production amount of the electrolyser, we can calculate how much power is required to compress it by multiplying the hydrogen production amount (*Var 2.23*) with the compression power requirement. Which is gained either from (*Eq. 3.6*) or (*3.12*) depending if one- or two-stage compression is used.

In part 4, the compression- and electrolyser consumption are summed together, and the result is the required power of the electrolysis process of one electrolyser. From this a new data, a vector with 24-hour intervals is created.

Important variables created in this part are:

Electrolysis_kWh	Electrolysis consumption [kWh/hour]	(Var 2.30)
Electrolysis_kWh_year	Total yearly consumption [kWh]	(Var 2.31)
Electrolysis_daily	Electrolysis consumption [kWh/day]	(Var 2.32)

3.3.5. Part 5-7: Excess energy & production

In the two scenarios this paper analyses, the primary electrolyser is accompanied by either a battery or a second electrolyser. A key factor in how efficient the system is overall is how the excess energy is utilized. The first step into finding out the utilizable amount of excess energy is deducting the electrolysis consumption from the total available energy, which is done in segment 5.

The sixth segment concentrates on the scenario where the electrolyser is accompanied by a battery. The battery is only used after PV energy is not enough to run the electrolyser. For this reason, daily values are used in excess energy for battery production, and daily results are gotten. If one were to use hourly values, MATLAB would calculate that the system has *BtCap* worth of kWh for every hour and as if the battery was used simultaneously with PVs. By using daily values, we can simulate a scenario where the battery is run during the night.

The available excess energy is limited according to the previously defined battery capacity. The production is again set to zero if it is insufficient for 10 % of the nominal production rate. We also determine how many days of the year the battery is not used at all and show this as *DNRB.*

Pexcess_usable	Hourly excess energy [kWh]	(Var 2.33)
Pexcess_usable_daily	Daily usable excess energy [kWh]	(Var 2.34)
H2batdaily_m3	H_2 produced with battery [m^3/day]	(Var 2.35)
H2batdaily_m3sum	Total H_2 produced with battery [m^3]	(Var 2.36)
H2batdaily_kg	H_2 produced with battery [kg/day]	(Var 2.37)
H2batdaily_kgsum	Total H_2 produced with battery [kg]	(Var 2.38)
NumOf_Cycles	# of battery cycles in one year	(Var 2.39)

Part seven repeats the previous task for the dual system. Hourly excess energy data (*Var 2.33*) is used because the second electrolyser can run simultaneously with the primary electrolyser. The days that the electrolyser is not running is shown as *DNR2* and the estimated hydrogen gas losses are deducted from the production amount.

H2excess_2ndelec	H_2 from the 2nd electrolyser [m^3/hour]	(Var 2.40)
H2excess_sum_m3	Total H_2 from the 2nd electrolyser [m^3]	(Var 2.41)
H2excess_kg	H_2 from the 2nd electrolyser [kg/hour]	(Var 2.42)
H2excess_sum_kg	Total H_2 from the 2nd electrolyser [kg]	(Var 2.43)
H2_2elec_daym3	H_2 from the 2nd electrolyser [m^3/day]	(Var 2.44)
Efficiency_Ely_2	Efficiency of the 2nd electrolyser	(Var 2.45)

3.3.6. Part 8-9: Unspent energy

In an optimum situation all the energy from the PV panels is used. But, especially with large PV installations like this, some of the energy is most likely left unspent. Part eight calculates the following variables for the two scenarios.

Unspent_bat	Unspent energy in a battery system [kwh/day]	(Var 2.46)
Unspent_batsum	Total unspent energy in a battery system [kWh]	(Var 2.47)
Unspent_elec	Unspent energy in a dual system [kWh/day]	(Var 2.48)
Unspent_elecsum	Total unspent energy in a dual system [kWh]	(Var 2.49)
H2unspent_batKG	Corresponding H_2 amount in a battery system [kg]	(Var 2.50)
H2unspent_elecKG	Corresponding H_2 amount in a dual system [kg]	(Var 2.51)

With these variables, MATLAB now creates a plot of the amount of energy that is left unspent in both scenarios and compares these two amounts to each other. Three more variables are created to help further comparison:

Prc_bat	How many % is left unspent in a battery system	(Var 2.52)
Prc_elec	How many % is left unspent in a dual system	(Var 2.53)
Pdiff	How many % more is left unspent in the least efficient option	(Var 2.54)

The percentual difference of the two systems is calculated with the following if-loop. By always dividing the larger variable with the smaller one, we can with a quick glance determine how much more energy would be wasted if we were to choose that option.

If *Prc_bat > Prc_elec*

$$Pdiff = \frac{Unspent\_batsum}{Unspent\_elecsum} * 100$$

else

$$Pdiff = \frac{Unspent\_elecsum}{Unspent\_batsum} * 100$$

end

3.3.7. Part 10: Total H_2 yield

After determining the separate hydrogen production amounts for the different components, in this part they are combined to enable further comparison. Firstly, the production amount in the battery system is calculated by combining the production from the primary electrolyser (*Var 2.23-26)* and the production that the battery is capable of (*Var 2.33-38*).

Then the variables of the battery system are replaced with variables from the dual system *(Var 2.40-44*) and the previous step is repeated. What is different, is that the data in the battery system has intervals of one day whereas the dual system data is given by each hour. Only the gravimetric production of the dual system is also transformed to daily values.

The final task done in this part is the creation of pie- and bar charts to visualize the results. The pie charts illustrate what proportion of the produced hydrogen is produced with the primary production method (electrolyser), secondary method (battery/electrolyser) and how much could still be produced if the system could use all available energy from the PV panels. The bar charts on the other hand indicate the total volumetric and gravimetric amounts of hydrogen produced with both systems.

3.3.8. Part 11: Utilization rates

Utilization rates for both systems are calculated following two strategies. In the first one, the maximum potential output of the systems is calculated with the assumption that they can be run non-stop even during the night. In the second one it is assumed the system only runs when there is sunshine for the PV panels. It is not known what is the absolute maximum production rate for different commercial electrolysers [25] , so openly disclosed nominal production rates are used for the calculations.

$$Capacity\ Utilization\ Rate = \frac{Actual\ output}{Potential\ output} \quad \text{(Eq. 3.15)}$$

Thus, in the first strategy the potential output is assumed to be $Output_{potential,max} = NPR_{1,2} * 24 * 365$. This assumes the electrolyser(s) can be run around the clock. The second principle on the other hand assumes that the electrolysers are only run during the hours of daylight. This results that the potential output is $Output_{potential,day} = NPR_{1,2} * DLH$ where DLH is the number of daylight hours in the year.

This part also calculates the average efficiencies for both electrolysers in the system.

3.3.9. Part 12: Timetables and results

Lastly the program complies all results into tables and timetables for further analysing. A summary of all of them can be found in '*Abbreviations_Dynamic.m*'. Timetables with hourly data are available for the dual system whereas for the battery system timetables with daily intervals are provided. In addition to these, the following two tables sum up the data for both systems.

TResultsElecBat	Summary of battery system	(Var 2.55)
TResultsTwoElec	Summary of dual system	(Var 2.56)

Parts 12.2 and 12.4 also have a loop that enable the user to see the storage tank level on each time interval. Lastly the file compiles all the results in the following excel files in the MATLAB folder.

SinglesystemHourly_Dynamic	Excel spreadsheet of the main electrolyser data
BatterysystemAll_Dynamic	Excel spreadsheet of the battery system data
DualsystemAll_Dynamic	Excel spreadsheet of the dual system data

3.4. Hydrogen storage

This MATLAB file (*Storage_H2.m*) is meant for a quick method to estimate how the storage tanks could be sized if the filling station is located on-site. The model consists of two storage tanks for different purposes.

Firstly, there is the low-pressure (ND) storage tank between the electrolyser and the compressor. Its purpose is to guarantee a uniform flow of gas to the compressor and the storage pressure varies between approximately 5 bars and 30 bars. After compression, the gas is stored momentarily in a storage tank of 300 bars (MD storage).

To calculate the necessary storage volume of the ND storage it is assumed that it is only required to have a storage bumper the size equal to the maximum volumetric production of hydrogen in any given hour. In our calculations we can utilize the ideal gas law, since in low pressures hydrogen behaves as such.

$$V_2 = \frac{P_1 * V_1}{P_2} \qquad \text{(Eq. 3.16)}$$

Where P_1 is the electrolysis pressure and P_2 is the compressor inlet pressure. V_1 equals the maximum amount of hydrogen in cubic meters produced at any moment during the year. Storage volume is calculated for two scenarios, one where production is done with a single electrolyser and another where two electrolysers are used.

VND1	ND volume for battery system [m^3]	(Var 2.57)
VND2	ND volume for dual system [m^3]	(Var 2.58)

Next, we assume that the MD storage tank can be emptied on regular intervals. We find out what is the maximum mass amount of hydrogen produced in a day in both scenarios and size the MD storage accordingly. The only variable in this file is how many days' worth of production the storage tank must be able to hold.

$$V_{MD} = m_{H2,max} * t \qquad \text{(Eq. 3.17)}$$

Where *m* is the maximum amount of hydrogen produced in one day (kg) and *t* is the time frequency of emptying the tanks (days). The high-pressure storage tank sizes are usually defined by how many kilograms of hydrogen they can hold and not by their volume as is done with the ND storage.

Days	# of days between emptying of the tanks	(Var 2.59)
MD1	Tank size for battery system [kg]	(Var 2.60)
MD2	Tank size for dual system [kg]	(Var 2.61)

It is worth noting that the timetables containing gravimetric production amounts also show the storage tank level according to (*Var 2.22*). This variable can be set according to the calculated storage tank size (*Var 2.60-61*) or, for example, to 500 kilograms, which is the usual limit of hydrogen transport lorries that can be used to transport the hydrogen to an external filling station.

4. System performance in different scenarios

This chapter demonstrates what outputs the MATLAB program can provide and compares different scenarios regarding electrolyser and battery sizes. Section 4.3. gives a quick look into the hydrogen refueling station and the pros and cons in different locations.

The system is located near Stuttgart, Germany, and it consists of 9 937 pieces of BenQ Solar PM060M02-290 Green Triplex -PV panels. The panels have an overall efficiency of 18%. They are orientated in a 20° angle and together cover 32 000 square meters of roof area. The optimum panels and their setup have been selected with Polysun software.

Panel type	BenQ Solar PM060M02-290 Green Triplex
# of panels	9 937
Area (m^2)	32 000
Declination	20°
Alignment	50% East / 50% West
Peak power	2 882 kWp
Produced per year	4 747 MWh

Table 4. Specifications of the PV setup

Because the main source of power are the PV panels, it is assumed that the more self-sufficient the system is, the better. This is why the utilization rates of the electrolysers are calculated with the assumption that only the hours of daylight are considered.

$$Capacity\ utilization\ rate = \frac{H_2\ produced}{Max\ H_2\ produced\ during\ daylight} \quad \text{(Eq. 3.18)}$$

The potential output of the electrolyser is thus estimated to be the amount produced if the electrolyser was running on full capacity only during the hours of daylight. With the available data this equals to 4 708 hours of the year. As summarized in table 5, hydrogen losses resulting from compression and decompression are in all scenarios assumed to be 5 %. The compressor electrical efficiency is set to 80 %. The general losses of the battery are assumed to be 10%. From electrolyser data [28] electrolysis itself is assumed to happen at 1 bar. All the electrolysers can achieve an output pressure of 30 bar with in-situ compression.

Electrolysis pressure	1 bar
Electrolysis temperature	80°C
Compressor efficiency	0,8
Compression temperature	50°C
Battery losses	10 %
Hydrogen gas losses	5 %

Table 5. Assumptions for all scenarios

For the results, the hydrogen is compressed from 30 bar to 300 bar with a two-stage compressor. It is assumed the compressor contains an intercooler, keeping the gas temperature at 50 degrees Celsius. With equations 3.1 – 3.3 the following Z-factors are achieved. The compression work required for each nominal cubic meter is calculated with equations 3.11 and 3.12.

P (bar)	**30**	**94,86**	**300**
T (°C)	Z_1	Z_m	Z_2
50	1,0201	1,0666	1,2352
W_{kWh}	0,1709 kWh/m^3		

Table 6. Compression variables for all scenarios

4.1. Analyzing different scenarios

This section analyses the results and tries to determine the most optimum sizing of components. To do so, four different scenarios are chosen, some with two electrolysers and some with an electrolyser and a battery.

4.1.1. Scenario #1: Large electrolyser and a battery

In scenario #1 the system consists of a large 2 MW electrolyser teamed up with a battery. The available battery capacity is set to 750 kWh which corresponds to about 1 500 kWh of installed capacity. This means that one full cycle equals a depth of discharge of 50 %.

Electrolyser model	nel Proton M400
Nominal power	2 MW
Type	PEM
H2 flow rate	413 Nm3/h
Power consumption	4,53 kWh/Nm3
Available battery capacity	750 kWh (1 500 kWh)
Feedwater consumption	373 l/h

Table 7. Scenario #1 spesifications

Firstly, we look at the hydrogen production rates achieved with the electrolyser and with the help of the battery. Figure 12 illustrates that the electrolyser is able to achieve a production rate of about 350 Nm^3/h almost throughout the year. This is behind its nominal production rate, most likely due to poor efficiency. In December and January, we see that the PVs cannot provide the system with enough energy to achieve the same peak production rates.

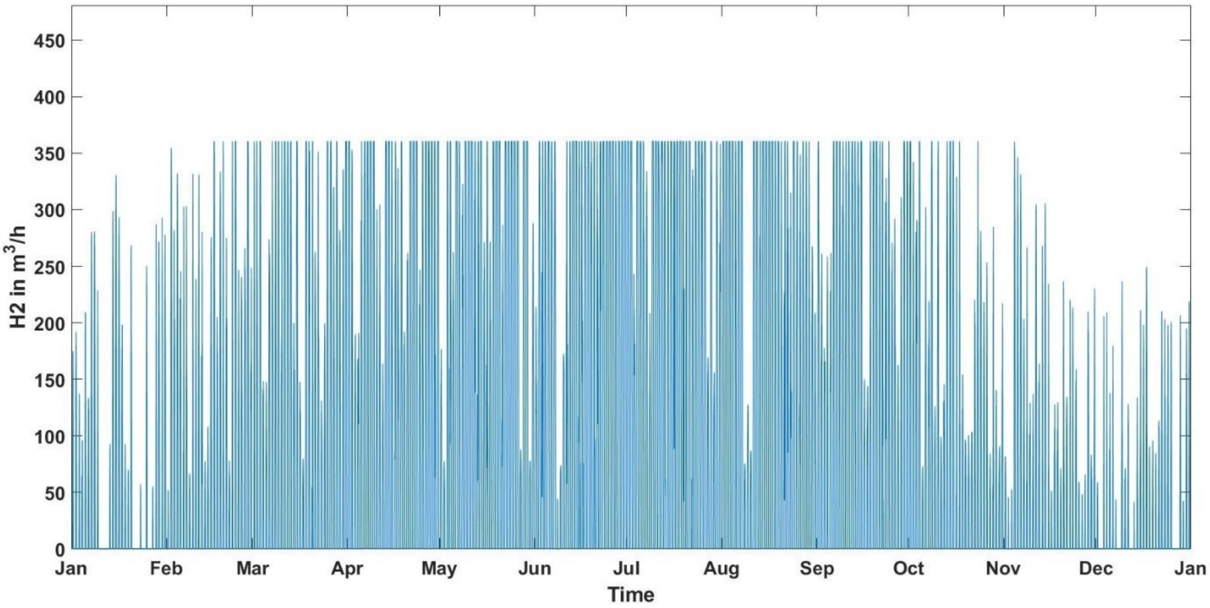

Figure 13. Volumetric H_2 production without battery in scenario #1

In total there are twelve days during the year that the electrolyser is not running without battery assistance, or in other words the PV output is not enough to meet the required power of the electrolyser which is 10% of its nominal production amount.

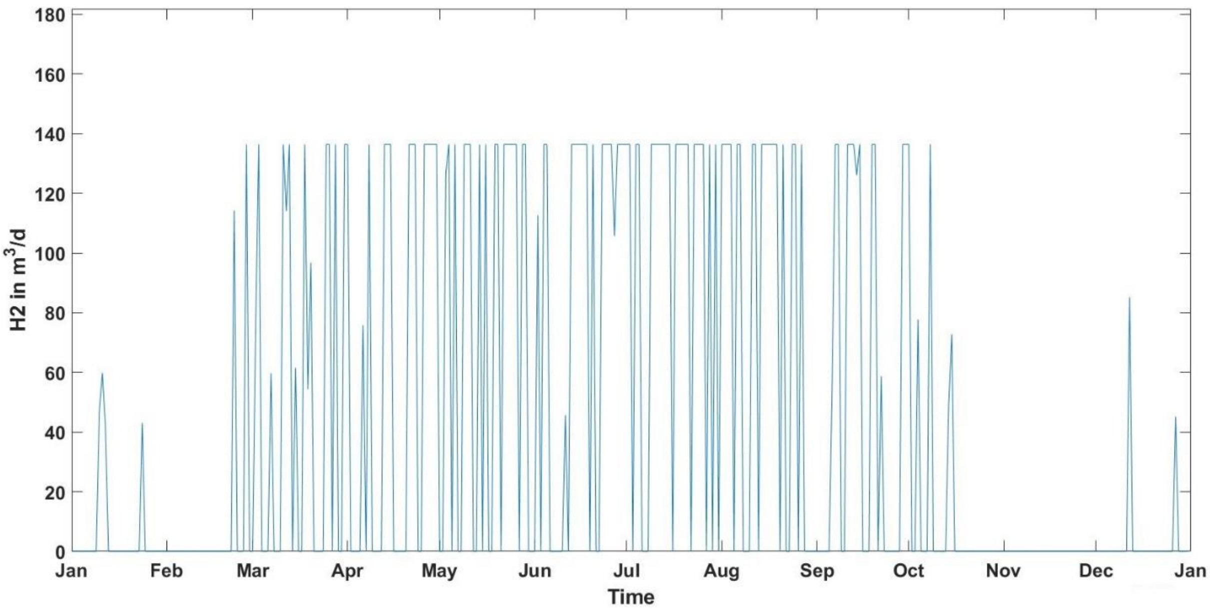

Figure 14. Volumetric H_2 production with battery capacity in scenario #1

With 750 kWh of available battery capacity we can reach a peak production of about 140 Nm^3 per day. And as shown by figure 13, we have a similar kind of production curve as in figure 12, with the exception that there seems to be close to no production between October and March. The battery is mostly used during the summer, with single peaks also in December and January. With a quick glance, the battery in this scenario seems like a bad investment due to long periods of non-operation.

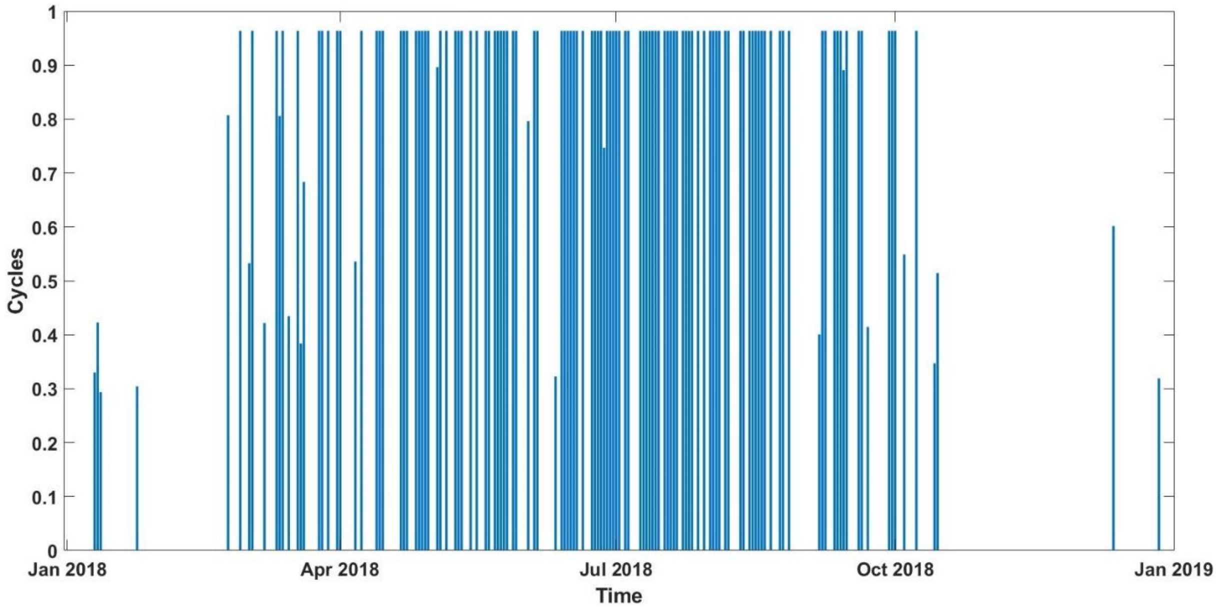

Figure 15. Battery cycles each day in scenario #1

Known reasons for Li-ion cell degradation are high rate of operation, cycling rate, temperature, operation on extended voltage levels, state of charge and depth of discharge [12]. As illustrated by figure 14, the battery in this system goes through 115 full cycles a year. The depth of discharge is 50 %. And as demonstrated by figure 15, the battery is only able to increase the hydrogen production by a small fraction. Because of this we conclude that the battery is not worth the investment in this system.

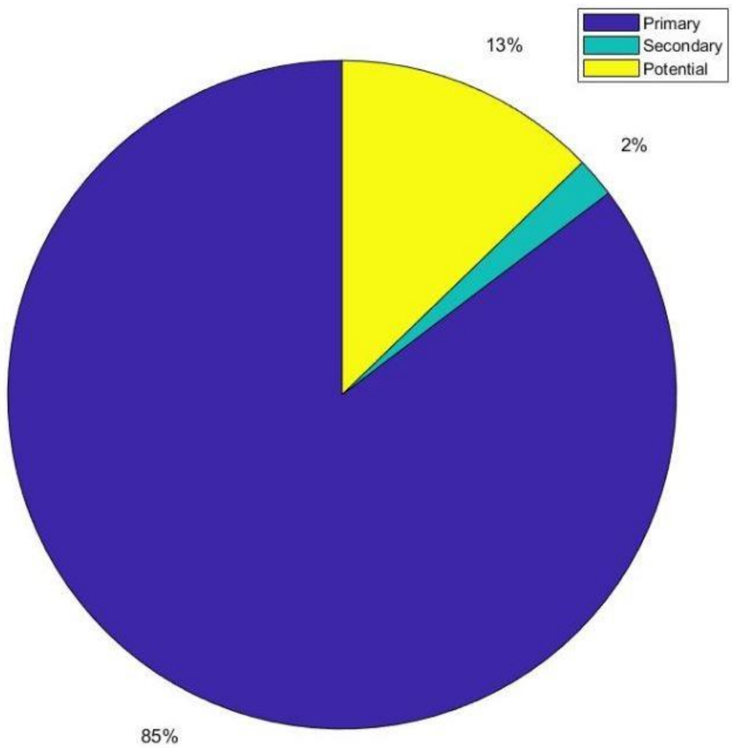

Figure 16. Hydrogen production distribution and amount that could still be produced in scenario #1

We see from figure 15 that most of the hydrogen (85%) is produced without the assistance of the battery and only 2% increase in production is done with the help of the battery capacity.

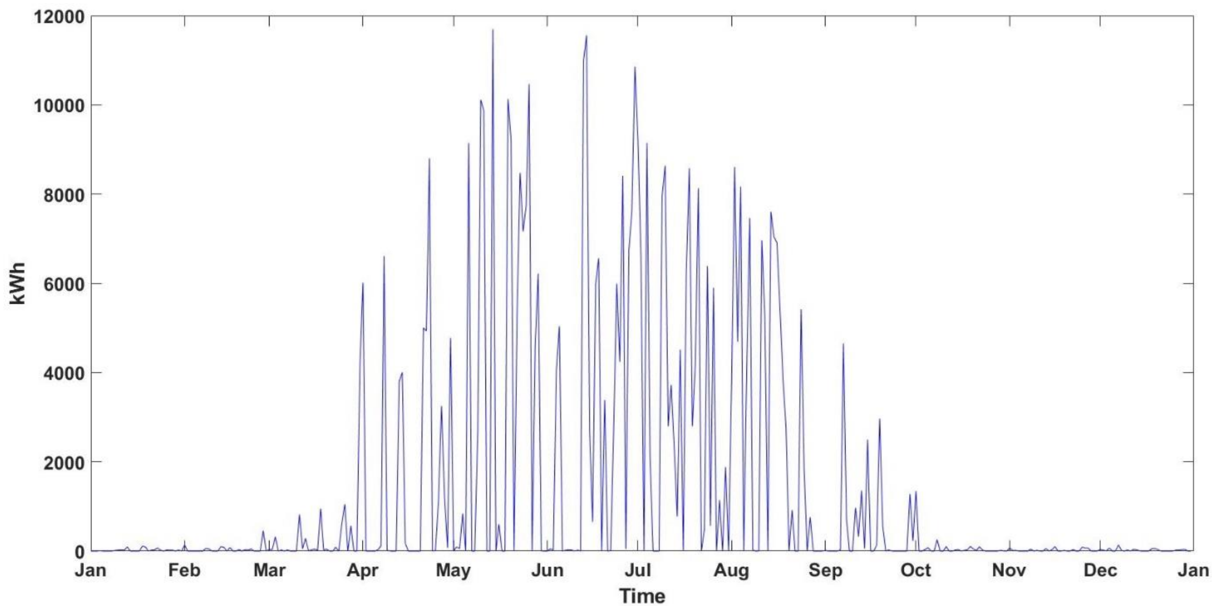

Figure 17. Unspent electricity for one year in scenario #1

The 10 % of electricity that is left for waste is distributed mostly during the summer months as shown in figure 16 and peaks around 12 000 kWh in June. The electrolyser requires a power input equal to 10 % of its nominal production rate, so in this case the electrolyser does not start unless it gets enough power to produce 41,3 Nm^3/h. From table 8 and figure 12 we can see that there are twelve days during which the PV output is not enough, and that the days are situated in December and January.

	Electrolyser	Battery	Total
H2 produced	49423	1116	50539
Days not running	12	235	
	Without battery	With battery	Cycles
Utilization rate	0,37	0,38	115
	% of total	kWh	
Unspent electricity	10,28 %	488 257	

Table 8. Summary of scenario #1 results

Because the battery is only used for a third of the year and produces so little hydrogen, and because aging tests using real operation conditions are very time- and cost intensive [29], this scenario is not selected.

4.1.2. Scenario #2: Large & small electrolyser

This scenario estimates if it would be better to replace the battery from the previous scenario with a small electrolyser. By using electrolysers from the same manufacturer we can expect lower maintenance costs.

Electrolyser models	nel Proton M400	nel Proton M100
Nominal power	2 MW	0,5 MW
Type	PEM	PEM
H2 flow rate	413 Nm3/h	103 Nm3/h
Power consumption	4,53 kWh/Nm3	4,53 kWh/Nm3
Feedwater consumption	373 l/h	< 200 l/h

Table 9. Scenario #2 spesifications

The main electrolyser is identical to the one in scenario one and figure 17 shows the hydrogen production of the electrolyser which is meant to replace the battery.

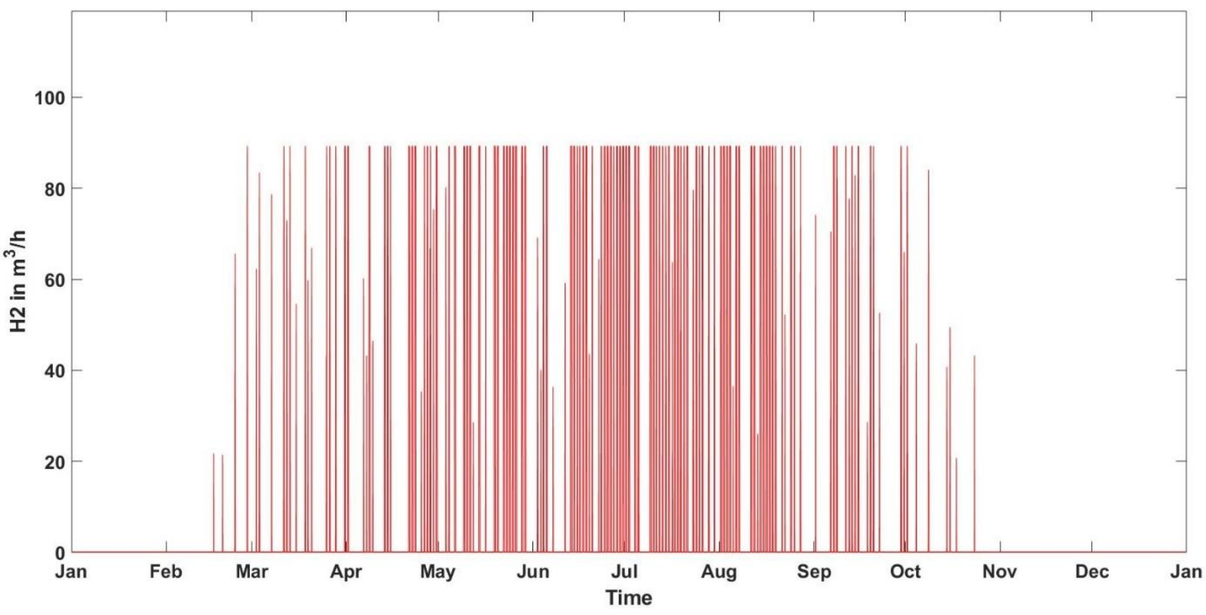

Figure 18. Secondary electrolyser volumetric production in scenario #2

We can see that the production chart is similar to that of the battery, with operation only between March and November. This indicates a very poor utilization rate, shown in table 10. In addition, the second electrolyser can only achieve production rate of 90 Nm^3/h.

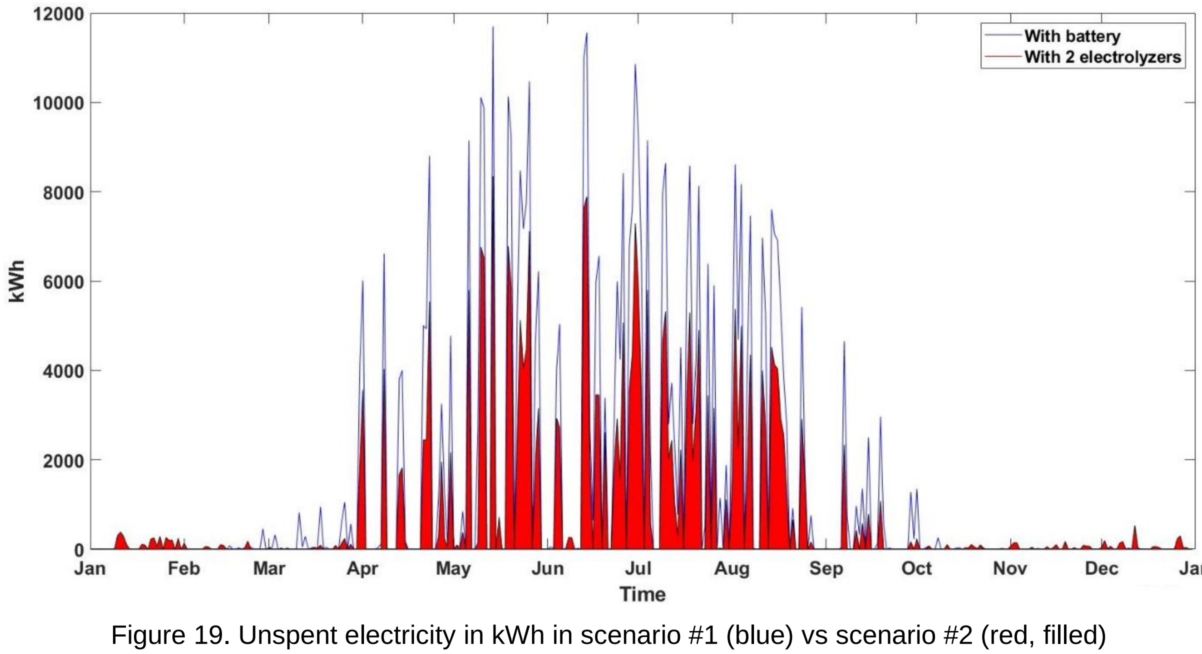

Figure 19. Unspent electricity in kWh in scenario #1 (blue) vs scenario #2 (red, filled)

From figure 18 we discern that providing the system with a second electrolyser instead of a battery is still not enough to take advantage of all the available energy from the PVs. The peak of lost electricity drops from 12 000 kWh/day to around 8 000 kWh/day. But even in the winter months there is some electricity going to waste due to the fact that it is not a sufficient amount to start the electrolysers.

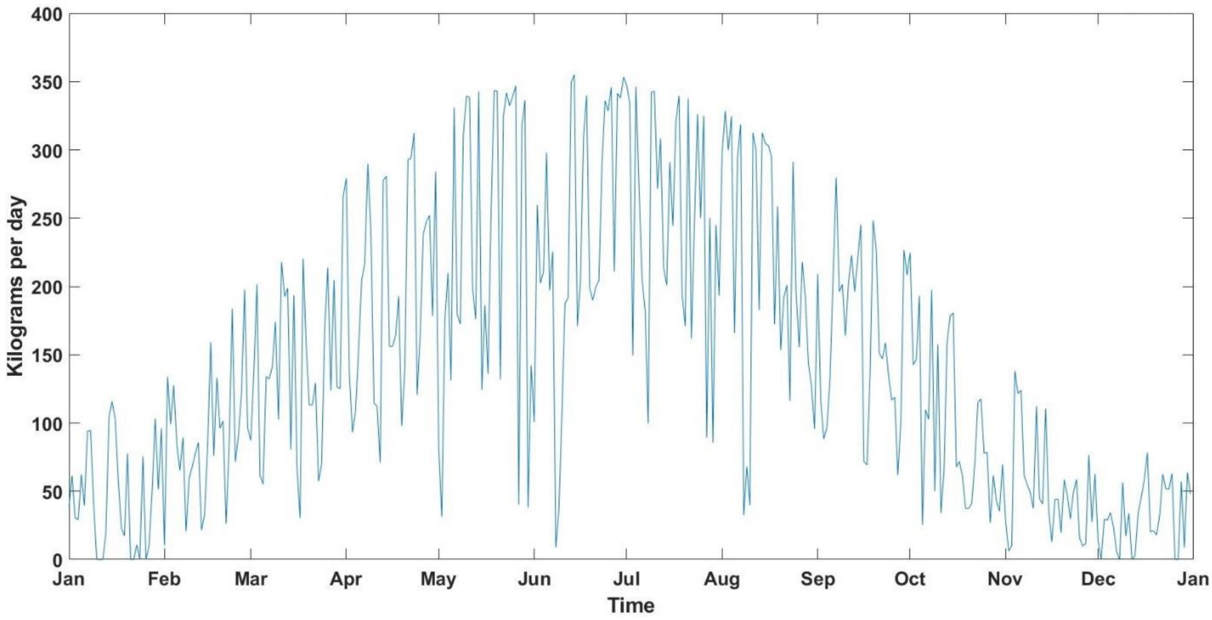

Figure 20. Gravimetric H2 production in scenario #2

As shown by the gravimetric production data, the monthly average in winter months such as December is well below 100 kg/day with some individual below-average days also in the summer months. The large variability of the production can be a problem, especially if the hydrogen is to be used by public or private mobility users that need a steady flow of fuel around the year. The most optimum situation would be a uniform production of H_2, but this might be impossible without a connection to the national electricity grid to guarantee production also in winter.

	Electrolyser #1	Electrolyser #2	Total
H2 produced (kg)	49423	3647	53070
Days not running	12	223	
Average efficiency	0,558	0,552	
	Electrolyser #1	Electrolyser #2	Total
Utilization rate	0,37	0,11	0,32
	% of total	kWh	
Unspent electricity	5,98 %	283 712	

Table 10. Summary of scenario #2 results

By looking at table 10 we can see that switching the battery to a small electrolyser provides us with close to 2 000 kg more hydrogen. Both the battery and the small electrolyser have over 200 days of non-operation during the year, thus achieving a very poor utilization rate. PEM electrolysers suffer from a high cost of components [16], so for this scenario to be feasible, the utilization rate should be increased for example with grid electricity. By fitting the system with a smaller primary electrolyser we can expect the electrolysers to have less non-operational days than in these scenarios.

4.1.3. Scenario #3: Two medium electrolysers

In this scenario we use two medium-sized, identical electrolysers without a battery. Again, by using two electrolysers from the same manufacturer we can expect lower maintenance costs of the system. We hope that using two electrolysers of equal size the utilization rate of the system can be improved from previous scenarios.

Electrolyser models	**2x** H-TEC ME 450/1400
Nominal power	**2x** 1 MW
Type	PEM
H2 flow rate	**2x** 210 Nm3/h
Power consumption	**2x** 4,9 kWh/Nm3
Feedwater consumption	**2x** 350 l/h

Table 11. Scenario #3 spesifications

We can expect the primary electrolyser have a much more uniform production rate also in the winter months due to the smaller required energy that the electrolyser needs to start. From figure 20 we can see that unlike with the large electrolyser (Fig. 12), we can now achieve the peak production rate also during the winter months.

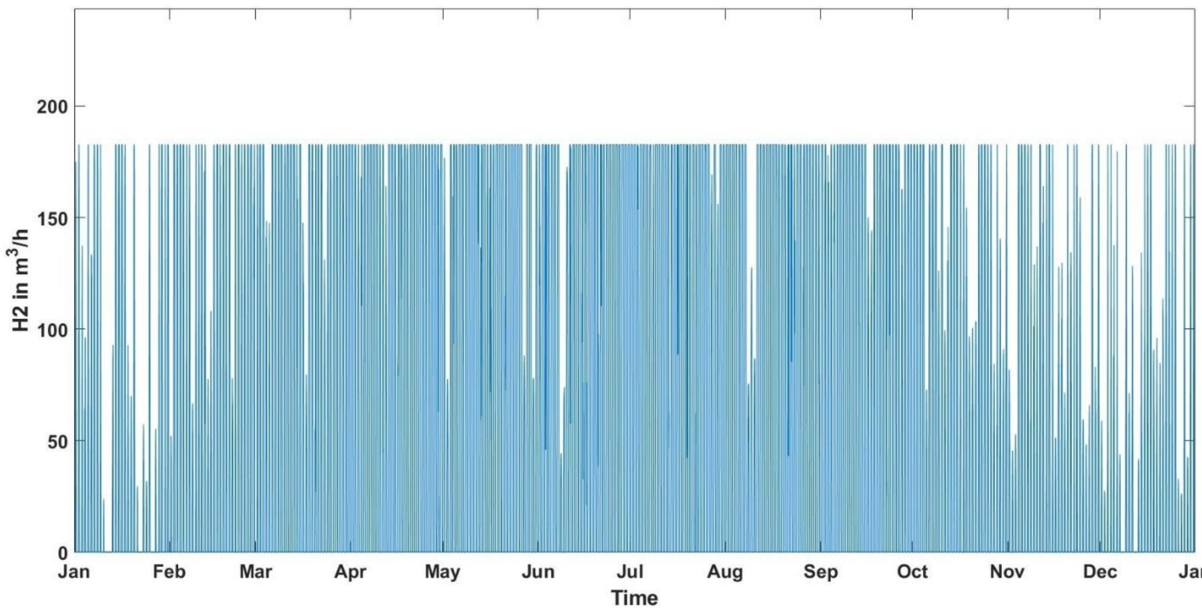

Figure 21. Primary electrolyser hourly production in one year in scenario #3

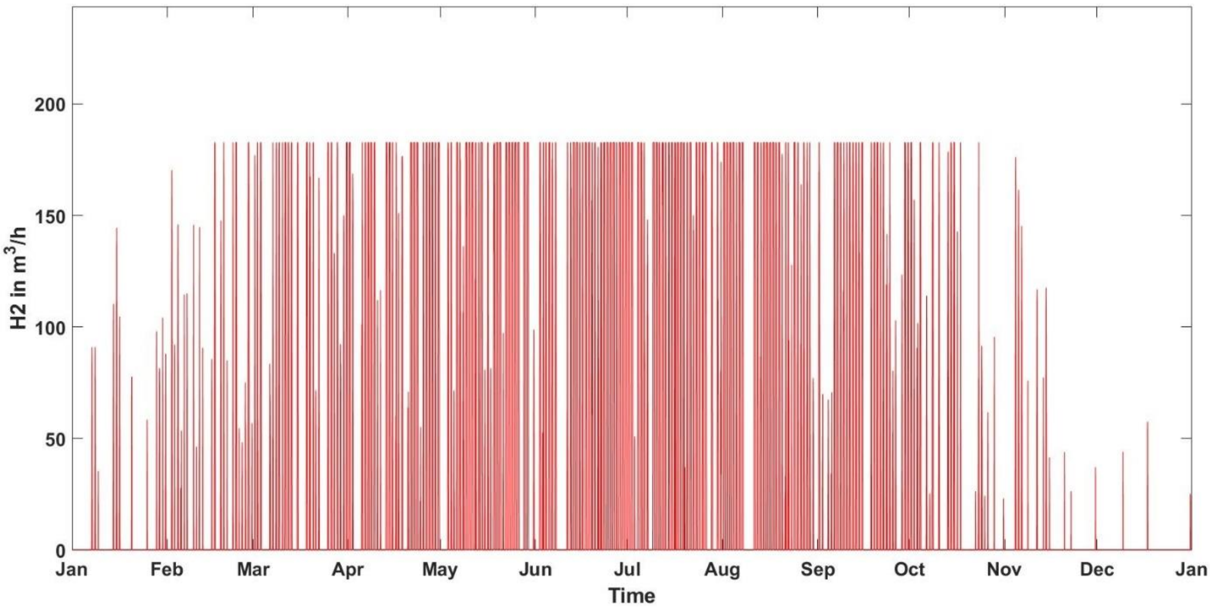

Figure 22. Secondary electrolyser hourly production in scenario #3

Figure 21 illustrates that we can expect a much worse utilization rate from the second electrolyser compared to the primary one, and a large number of days of non-operation in the winter months. Yet it is clear this option is much better as a secondary solution than the ones offered in the previous scenarios (Fig. 13 & Fig. 17). The production is also much more evenly split between both electrolysers as shown in figure 22. This makes the second equally sized electrolyser a much worthwhile investment than the battery or the small electrolyser from previous scenarios.

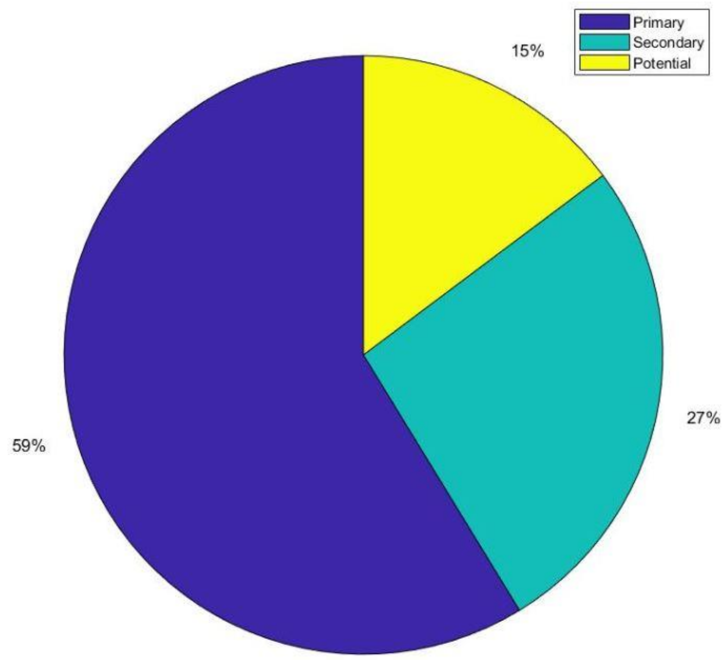

Figure 23. Hydrogen production distribution and amount that could still be produced in scenario #3

The primary electrolyser has a superior utilization rate compared to the other scenarios as shown in table 12, and the utilization rate of the second electrolyser can be improved by running the electrolyser(s) with additional off-peak electricity. In December 2018 and January 2019, the rough average price of off-peak electricity was about 50 €/MWh [30].

Even though a slightly bigger portion of electricity is left unspent, hydrogen production amount is almost as large as in previous scenarios. And due to the high utilization rate of the first electrolyser, this scenario seems like the most optimum one. The average efficiencies of both electrolysers are also slightly better in this scenario rather than the previous one.

	Electrolyser #1	Electrolyser #2	Total
H2 produced (kg)	34256	15462	49718
Days not running	6	113	
Average efficiency	0,560	0,562	
	Electrolyser #1	Electrolyser #2	Total
Utilization rate	0,50	0,23	0,37
	% of total	kWh	
Unspent electricity	12,94 %	614 490	

Table 12. Summary of scenario #3 results

4.1.4. Scenario #4 Medium electrolyser with battery

Because the cost of components in PEM electrolysis is high [16], it might be more feasible to use a battery instead of a second electrolyser to drive up the system utilization rate. The final scenario will use an identical electrolyser from the previous scenario coupled with a 1 500 kWh battery which has 750 kWh of available capacity (with assumed depth of discharge of 50 %).

Electrolyser models	H-TEC ME 450/1400
Nominal power	1 MW
Type	PEM
H2 flow rate	210 Nm3/h
Power consumption	4,9 kWh/Nm3
Feedwater consumption	350 l/h
Battery capacity	750 kWh (1 500 kWh)

Table 13. Scenario #4 specifications

With figure 23 we can compare how well the battery performs when compared with a second electrolyser (Fig. 21). The battery seems to achieve higher production rates also in December and January, which is something the second electrolyser in Fig. 21 cannot do.

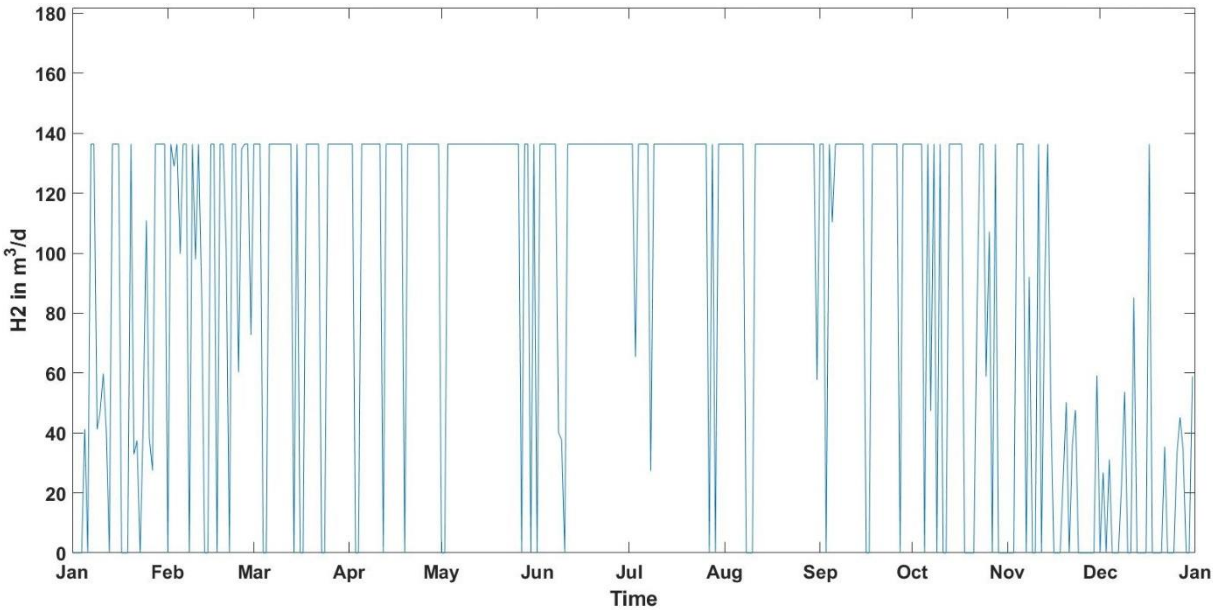

Figure 24. Volumetric H_2 production with battery capacity in scenario #4

As mentioned earlier, multiple variables have an effect on Li-ion cells degradation rate, cycling rate being one of them. Barré [31] concludes that real life estimation of the battery life without actual experiments is nigh impossible and that “*there is currently no study considering ageing as a consequence of all the existent interactions between environment and utilization mode*”.

But in a study by Bryden [12], after 400 cycles the Li-ion battery capacity was around 80% of the original capacity. As shown in figure 24, the battery in this system would go through 248 cycles within one year, thus rapidly shortening its lifespan meaning it would have to be replaced more often.

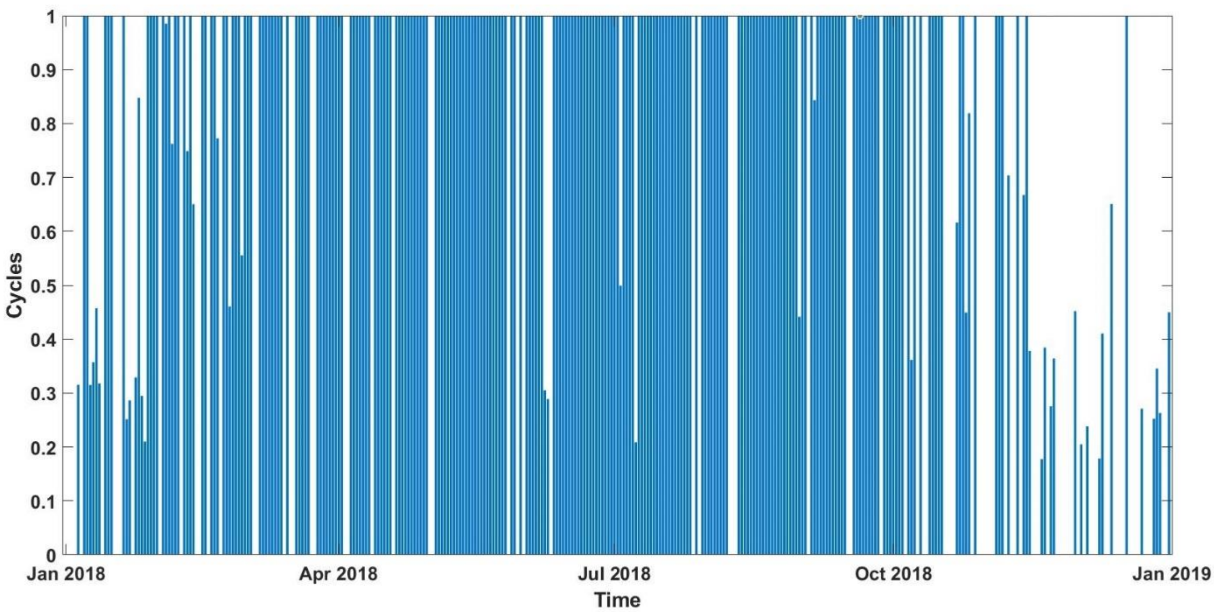

Figure 25. Battery cycles each day in scenario #4

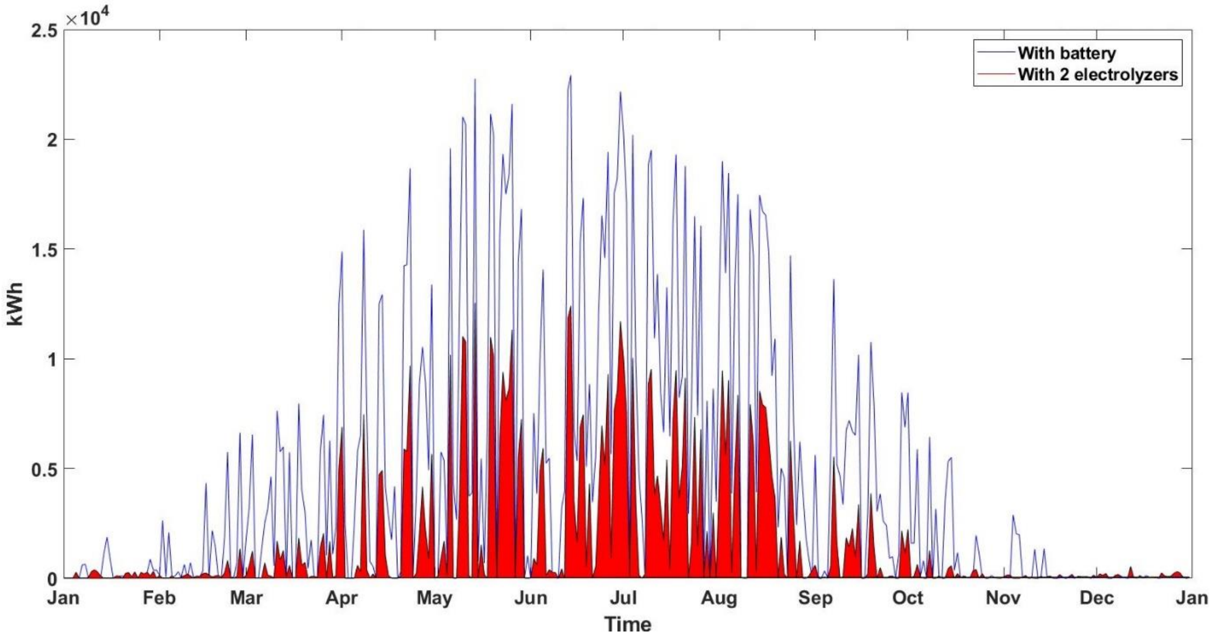

Figure 26. Unspent electricity in scenario #4 (blue) compared to #3 (red, filled)

High cycling rate together with a larger portion of wasted electricity (Fig. 25), shows that this scenario is not an improvement and replacing the second electrolyser is not a feasible option and thus we choose scenario #3 as our optimum system model.

	Electrolyser	Battery	Total
H2 produced	34256	2318	36574
Days not running	6	91	
	Without battery	With battery	Cycles
Utilization rate	0,50	0,54	248
	% of total	kWh	
Unspent electricity	35,83 %	1 701 380	

Table 14. Summary of scenario #4 results

4.2. Summary of the chosen scenario

The chosen sizing of components is decided as having two medium sized electrolysers without a battery. A medium sized primary electrolyser has a superior utilization rate compared to a bigger one and the second electrolyser produces significantly more hydrogen than would be possible to produce with a battery. A battery would also suffer from a high cycling rate which in turn would decrease its lifespan significantly faster than what is reasonable.

Electrolyser models	**2x** H-TEC ME 450/1400
Nominal power	**2x** 1 MW
Type	PEM
H2 flow rate	**2x** 210 Nm3/h
Power consumption	**2x** 4,9 kWh/Nm3
Feedwater consumption	**2x** 350 l/h

Table 15. Optimum scenario specifications

	Electrolyser #1	Electrolyser #2	Total
H2 produced (kg)	34256	15462	49718
Days not running	6	113	
Average efficiency	0,560	0,562	
	Electrolyser #1	Electrolyser #2	Total
Utilization rate	0,50	0,23	0,37
	% of total	kWh	
Unspent electricity	12,94 %	614 490	

Table 16. Optimum scenario summary of results

Next, we take a look at the production and related storage tank level for one winter week and one summer week to estimate how often the hydrogen would need to be transported to a filling station.

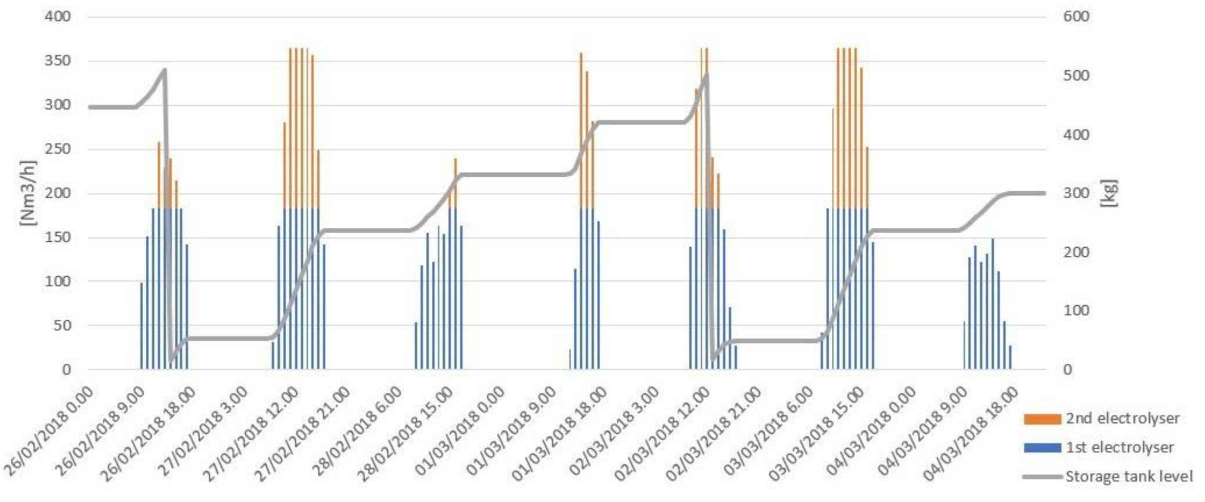

Figure 27. Hydrogen production in relation to storage tank level, winter week (one spike equals one hour)

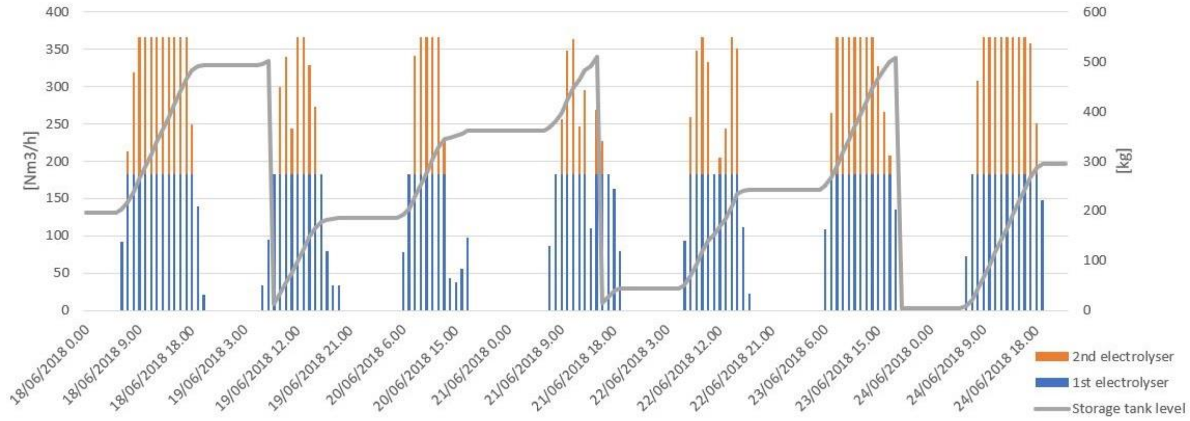

Figure 28. Hydrogen production in relation to storage tank level, summer week (one spike equals one hour)

By comparing the winter production (Fig. 26) with production in the summer (Fig. 27), we see that when the storage tank level is set to 500 kilograms, we would require a hydrogen transport lorry on average twice a week. Whereas during summer it would require transporting the hydrogen three, sometimes four, times a week. Tube trailers most commonly have a transport capacity of 500 kilograms but by using a container trailer, this can be increased to 1000 kilograms [13] thus decreasing our transport needs and costs. From figure 26 we also see the reason for the poor utilization rate of the second electrolyser: for example, on 28/02 the second electrolyser is in operation only for two hours. In the summer it is used simultaneously with the first one during almost every hour.

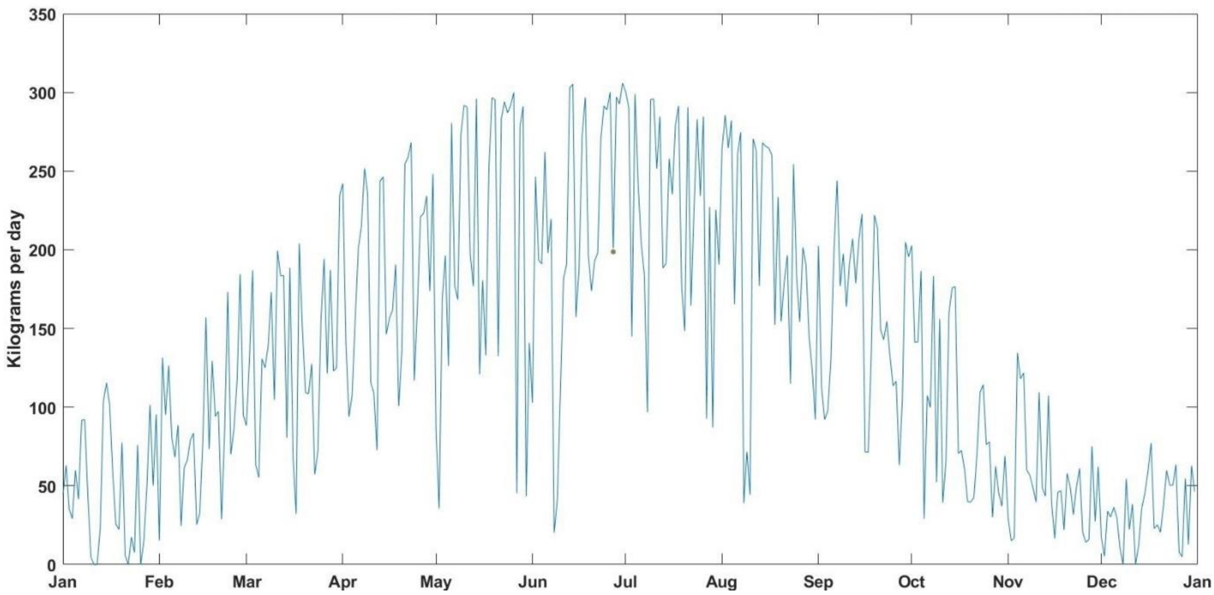

Figure 29. Gravimetric daily H_2 production in optimum scenario

As demonstrated by figure 29, the daily production of hydrogen does not even reach an average of 50 kilograms per day in the winter. Starting from November all the way until February, we have very low production amounts. Hydrogen busses carry approximately 30 - 50 kilograms of H_2 on board. And newer busses consume 8 – 9 kg/100km [13]. Small variation in the production is not a problem. The refuelling schedule of the busses can be arranged to accommodate this variation. But in the winter months the production is still unacceptably low and not enough to supply an entire bus fleet. This is another reason to improve the utilization rate of the electrolysers with electricity from the power grid.

4.3. Hydrogen delivery and refuelling station

One major obstruction to the spread of hydrogen fuel cell vehicles (HFCVs) is the lack of hydrogen refuelling station infrastructure. To achieve the favour of consumers, hydrogen needs to be competitively priced and conveniently available. The location of the hydrogen refuelling stations affects the hydrogen life cycle cost and the price of hydrogen [32]. That is why their placement should be carefully considered to ensure that the hydrogen demand is met. Having the hydrogen station on-site would create cost savings in the transportation to the refuelling station. But if also passenger HFCVs, not only busses, would use this refuelling station, it’s location might push consumers away.

Gaseous hydrogen can be transported to the refuelling station either by compressed pressure vessels or via a pipeline. Using compressed pressure vessels and transporting the hydrogen with tube trailers is usually the simplest method in terms of infrastructure requirements. Tube trailers also have very small hydrogen losses and the compression cost at the refuelling station is low [33]. Capital costs of transport trucks are around ~300.000 USD ($) per truck with additional operating costs of around 0,10 – 0,40 $/kg. Total operating costs would thus be 0,5 – 2,0 $/kg/100 km [34].

Using traditional pipelines, i.e. pipelines such as those for natural gas, is capital intensive and require large quantities of gas [34] and thus is not suitable for a situation such as this where production amounts are low. Capital costs for hydrogen pipeline have a large variation, from 200.000 – 1.000.000 $ per kilometre. Total costs of operation can still be very low, around 0,10 – 1,00 $/kg/100km [34].

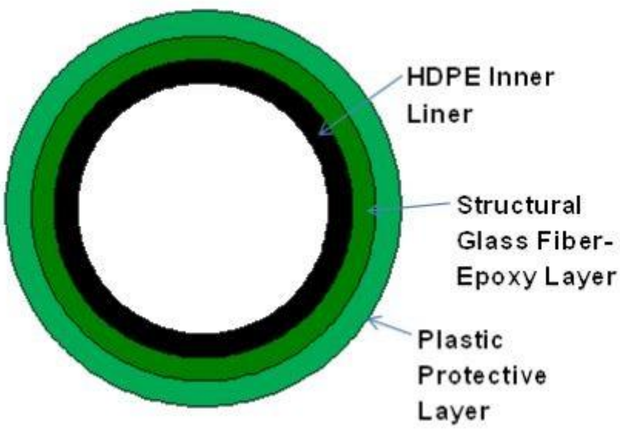

Figure 30. FRP pipeline cross section [35]

Hydrogen embrittlement is a concern with steel materials. Instead of using steel materials, one potential pipeline material is Fiber Reinforced Polymer (FRP), shown in figure 29. The installation of FRP pipelines is less labour-demanding and requires less heavy machinery. This lowers the installation costs by up to 30 % [33].

The customer in this case is the public transportation fleet of the Stuttgart area, i.e. hydrogen busses. Because the customer is a single entity, there is less pressure the consider the positioning of the refuelling station. By having the hydrogen refuelling station on-site, cost-savings in hydrogen transportation are achieved. If the hydrogen would also be sold for private passenger cars, we would have to position the refuelling station as close to the consumer as reasonably possible.

5. Summary and outlook

5.1. Summary

Due to the unchecked use of fossil fuels, we are now facing a multitude of environmental problems. Hydrogen is widely seen as a fuel of the future that will help societies get rid of their fossil fuel dependency. In answer to this, a solar-fed power-to-gas plant will be built in an industrial area near Stuttgart. There photovoltaic panels will cover a roof area of approximately 32 000 square meters. This energy is then used to create hydrogen in a PEM electrolyser. The hydrogen is then used by the public transports' bus fleet.

The purpose of this paper is to create a MATLAB modelling tool that will help in sizing the components. The MATLAB tool consists of multiple files, and there are separate files for different stages of the process. After comparing different scenarios, the best combination of components one is chosen. It is found that equipping the system with a battery would provide only a marginal increase in hydrogen production. In addition, the battery degradation rate will increase if it goes through too many cycles during a year. For these reasons, a system with two electrolysers is chosen.

As the most optimum scenario, two H-TEC ME 450/1400 electrolysers are selected. By using two 1 MW electrolysers, we reach utilization rates of 50 % and 23 % with a total hydrogen production of almost 50 000 kilograms. All available energy from the PVs cannot be utilized, with 600 000 kWh (13 %) being unspent. It is advisable that the utilization rates of both electrolysers are improved by using off-peak electricity, especially during the winter months when production is low. The hydrogen refuelling station is recommended to have on-site, because the customers are only the HFC busses belonging to the public transport fleet.

5.2. Outlook

Future research might attempt to use more sophisticated methods in sizing the components. One such possible way could be using the HOMER energy software that evaluates the different components and chooses the most economical and technological combination of components, and then performing a multi-year performance analysis with TRNSYS software as done by [36].

A possible improvement would also be a more thorough model of the battery degradation rate. The battery loses its capacity according to the number of cycles it goes through. Implementing this degradation rate would help evaluate the battery efficiency better. Detailed calculations about the costs of running the system with off-peak electricity would also benefit this work. These calculations could also include what would be gained if the unspent electricity from the summer months is sold to the national electricity grid. Or perhaps an energy management system can increase the utilization rates.

Doubts may also be raised as to whether the compressibility factor calculations provided by Babel [22] are completely correct. Previous studies, such as those by Makridis and Zhou et al. [20, 37, 38], suggest that the compressibility factors are smaller than those in this paper. Yet problems arise because the values provided in previous studies also contradict each other. Online data by LBS GmbH [38] does not provide calculations. A book by Hirscher [39] on the other hand is not available as open-access. A study by Tzimas et al. [18] provides different values even within one paper. So, despite there being a substantial body of literature on the subject, a consensus on the correct compressibility factor is almost impossible to discern.

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