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HYCONOMICS

TECHNICAL-ECONOMIC STUDY OF A HYDROGEN FACTORY

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José Albano Alves Araújo

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EFACEC

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Abstract

The world faces one of its greatest challenges - climate change, with all its harmful repercussions. For several years now, this issue has been gaining notoriety, and awareness actions, demonstrations and protests have been converted into international agreements led at summits. The Paris Agreement, negotiated during the COP21 (United Nations Climate Change Conference 2015) is an example. The agenda is then put to practice through new policies, across all member states.

It is in this context that hydrogen appears, not only as an energy vector, but also as a feedstock in various chemical processes and fuel. The total hydrogen market today is ca. 70 Mton. There are several ways of producing it, with different levels of carbon dioxide emissions associated. The most popular method is through Steam Methane Reform (SMR) which corresponds to “grey hydrogen” as further discussed in section 1. Hydrogen produced from water electrolysis accounts for ca. 4 % of the total amount produced today worldwide.

It was possible to phenomenologically model an electrolyser to simulate the production of a hydrogen stream in SimulationX, a simulation platform with object-oriented language, Modelica. The values for the cell voltage and current density were 1.82 V and 2.19 $A \cdot cm^{-2}$, respectively. As for the mass flow a value of 406.8 $kg \cdot h^{-1}$ was achieved for an electrolyser power of 20 MW. Regarding the financial results for the project, the net present value of the investment was calculated for two distinct scenarios. Considering a hydrogen selling price of 2.70 $€ \cdot kg^{-1}$, resulted in losses, ranging from 15 M€ for alkaline electrolysis and 30 M€ for PEM electrolysis; for selling prices of 4 $€ \cdot kg^{-1}$ only the alkaline technology is profitable while for 5.5 $€ \cdot kg^{-1}$ alkaline and PEM electrolyser technologies are profitable.

Keywords: Hydrogen, Green Hydrogen, Renewable Energy, Electrolyser, Simulation.

Resumo

O mundo enfrenta um dos seus maiores desafios - as alterações climáticas, com todas as suas repercussões nocivas. Há vários anos que esta questão tem vindo a ganhar notoriedade, e as ações de sensibilização, manifestações e protestos têm sido convertidas em acordos internacionais protagonizados em cimeiras. O Acordo de Paris, negociado durante a COP21 (Conferência das Nações Unidas sobre Alterações Climáticas de 2015) é um exemplo. A agenda é então posta em prática através de novas políticas, em todos os estados-membros.

É neste contexto que o hidrogénio aparece, não só como um vetor energético, mas também como uma matéria-prima e combustível. O mercado total de hidrogénio hoje em dia é de cerca de 70 Mton. Há várias formas de o produzir, com diferentes níveis de emissões de dióxido de carbono associadas. O método mais popular é através da Reforma do Metano a Vapor, que corresponde ao "hidrogénio cinzento", tal como discutido mais detalhadamente na secção 1. O hidrogénio produzido a partir da eletrólise da água corresponde a cerca de 4 % da quantidade total produzida atualmente a nível mundial.

Foi possível modelar fenomenologicamente um eletrolisador para simular a produção de hidrogénio em SimulationX, uma plataforma de simulação com linguagem orientada a objetos, Modelica. Os valores de operação de voltagem e densidade de corrente foram de 1,82 V e 2,19 $A \cdot cm^{-2}$, respetivamente. Quanto ao fluxo de massa, foi alcançado um valor de 406,8 $kg \cdot h^{-1}$ para uma potência do eletrolisador de 20 MW. Quanto aos resultados financeiros do projeto, o valor atual líquido do investimento foi calculado para dois cenários distintos. Considerando um preço de venda de hidrogénio de 2.70 $€ \cdot kg^{-1}$, o resultado foi negativo, resultando em perdas, variando entre 15 milhões de euros para a eletrólise alcalina e 30 milhões de euros para a eletrólise PEM; para preços de venda de 4 $€ \cdot kg^{-1}$ apenas a tecnologia alcalina é rentável, enquanto para 5.5 $€ \cdot kg^{-1}$ as tecnologias alcalinas e PEM são ambas rentáveis.

Palavras-Chave: Hidrogénio, Hidrogénio Verde, Energias Renováveis, Eletrólise, Simulação.

Declaration

I hereby declare, under word of honour, that this work is original and that all non-original contributions are indicated, and due reference is given to the author and source

(José Albano Alves Araújo)

Porto, 4th of July 2021

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Notation and Glossary

ΔH	Change in enthalpy	$J\cdot mol^{-1}$
ΔG	Change in Gibbs free energy	$J\cdot mol^{-1}$
T	Temperature	K
ΔS	Change in entropy	$J\cdot mol^{-1}K^{-1}$
E^0	Thermoneutral voltage	V
z	Number of transferred electrons	
F	Faraday constant	$C\cdot mol^{-1}$
E_{cell}	Cell's operation voltage	V
E_{therm}	Thermodynamic potential	V
η_{act}	Activation overpotential	V
η_{ohmic}	Ohmic losses	V
E_{rev}	Reversible Potential	V
R	Universal gas constant	$J\ mol^{-1}\ K^{-1}$
P_i	Partial pressure	bar
i	Theoretical current density	$A\cdot cm^{-2}$
i_0	Exchanged current density	$A\cdot cm^{-2}$
σ_{m}	Membrane conductivity	$S\cdot cm^{-1}$
R_m	Membrane resistance	Ω
t_m	Membrane thickness	μm
A_{cell}	Area of the cell	cm^2
η_F	Faraday's efficiency	
n	Number of mols	mol
M	Molar mass	$g\cdot mol^{-1}$

Greek Letters

α	Transfer coefficient
λ	Membrane water content
σ	Membrane conductivity

Indexes

a	anode
c	cathode
m	membrane

List of Acronyms

COP21	United Nations Climate Change Conference 2015
UE27	European Union
SMR	Steam Methane Reform
CCS	Carbon Capture and Storage
IRENA	International Renewable Energy Agency
PV	Photovoltaics
VRE	Variable Renewable Energy
GHG	Green House Gases
KPI	Key Point Indicator
AEM	Anion Exchange Membrane

PEM	Proton Exchange Membrane
PGM	Platinum Group Metals
HHV	Higher Heating Value
OER	Oxygen Evolution Reaction
HER	Hydrogen Evolution Reaction
VPSA	Vacuum Pressure Swing Adsorption
MIBEL	Iberian Electricity Market
OMI	Iberian Market Operator
OMIP	Iberian Market Operator – Portuguese section
OMIE	Iberian Market Operator – Spanish section
NPV	Net Present Value
OPEX	Operation Expenditures
CAPEX	Capital Expenditures
EBITDA	Earnings Before Interests, Taxes, Depreciation and Amortization
CF	Cash-Flow

1 Introduction

1.1 Framing and presentation of the work

With the Paris Agreement signed on the 4th of November 2016, the international community seeks for a global and effective response to the urgent need to halt the increase in the global average temperature [1]. One of the central objectives on this agreement is to limit the increase of the global average temperature below 2 °C this century, highlighting the need to use renewable energy sources to decarbonize the energy. “Green Hydrogen” is expected to play a major role as energy and feedstock during this energy paradigm transition.

It is therefore convenient to categorise and distinguish the different “shades” of hydrogen as well as their meaning. Hydrogen can be produced by various processes and using different energy sources, hence, a colour code has been created to facilitate rapid identification of the type of hydrogen, taking into account the intensity of released CO_2 to the atmosphere – Figure 1.

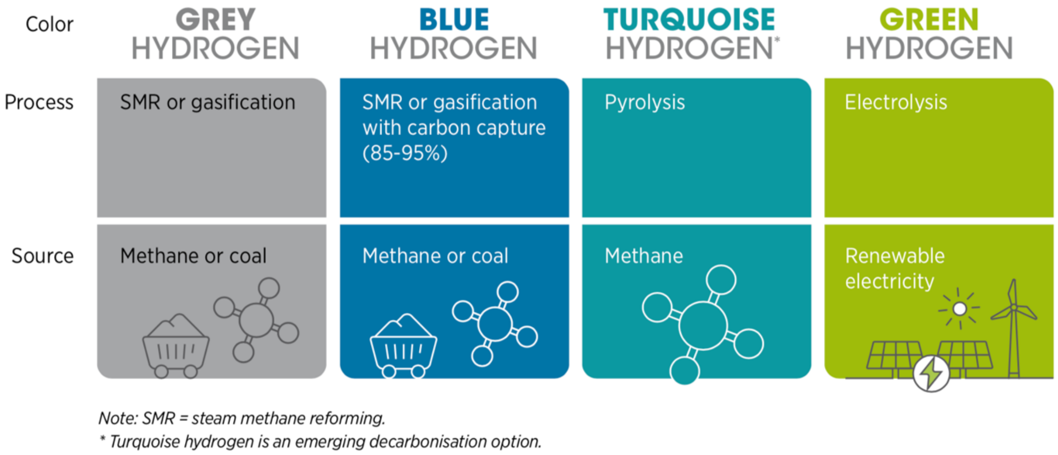


Figure 1 - Hydrogen colour code (extracted from [2])

“Grey Hydrogen” is produced from steam methane reforming or from coal gasification. Thus, the use of this type of hydrogen entails a substantial amount of CO_2 emissions to the atmosphere.

“Blue Hydrogen” consists of the same process as before but coupled with a CO_2 capture and sequestration system (CCS – Carbon Capture and Storage) with a capture efficiency of ca. 85-95 % [2]. The blue hydrogen produces more CO_2 and consumes more fossil fuel than grey hydrogen; however, this CO_2 is prevented from reaching the atmosphere since it is captured and stored.

“Turquoise Hydrogen” is produced by methane decomposition either of natural gas or biomethane, where methane is decomposed into solid carbon and hydrogen. This technology is still at pilot stage [3]. When biomethane is used, the methane decomposition removes CO_2 from the atmosphere at competitive costs.

Finally, “Green Hydrogen” is produced through the water electrolysis relying exclusively on renewable electricity, neither producing nor emitting CO_2.

There are several factors that contribute to the implementation of hydrogen-based technologies. In the past, hydrogen has already been on the spotlight due to drastic and unexpected oil price rises as it could bridge this demand-side imbalance in the energy market, once it considers new and diversified markets, producers and supply chains. This contributes to greater energy security and increases the overall system resilience. The fact that it can be used as a non-polluting fuel when combined with a fuel cell also makes it very attractive. Moreover, in a macroeconomic analysis, it can promote job creation and economic growth for a country [2].

Nonetheless, there are more specific features that will make “Green Hydrogen” more attractive.

1.1.1 Decreasing costs of renewable electricity

With the growing share of energy from renewable sources its cost has been considerably reduced as illustrated in Figure 2.

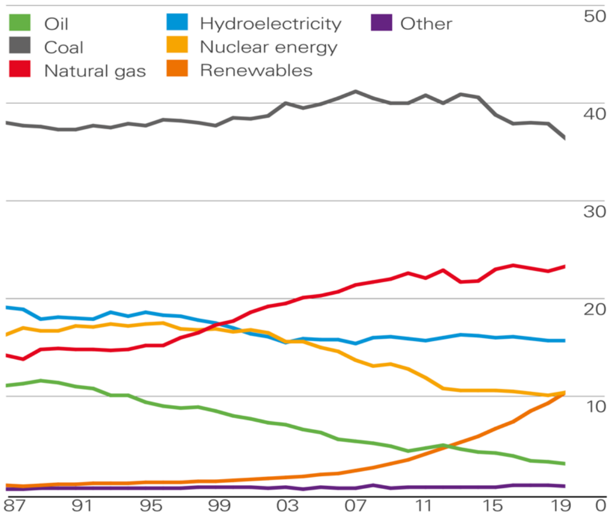


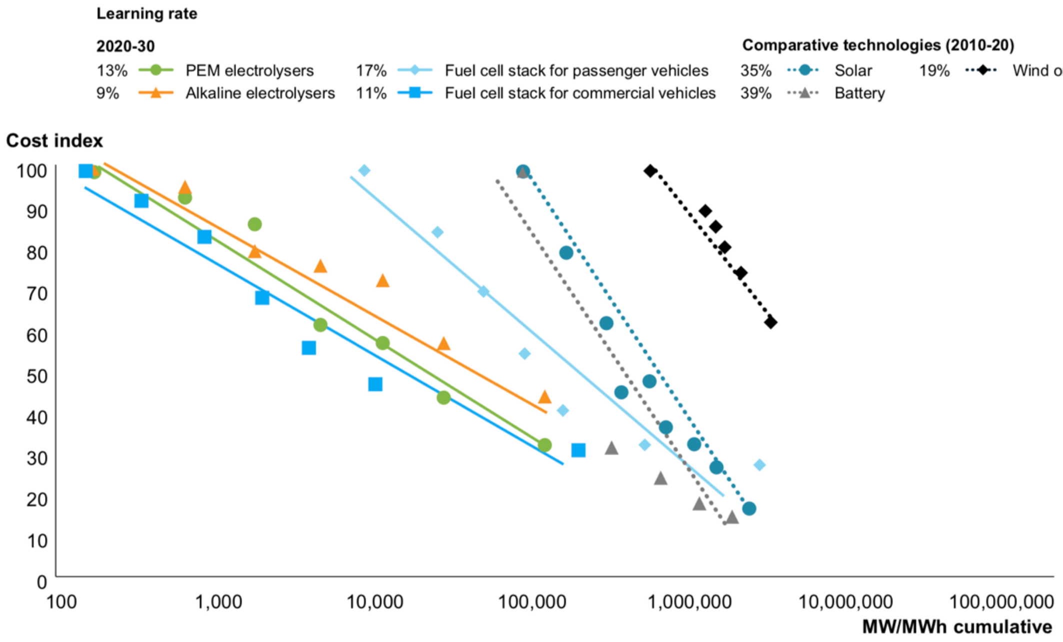
Figure 2 - Share of global electricity generation by fuel (extracted from [4])

The share of renewables (dark orange line) seems to be assuming an exponential function shape. This means that the overall investment costs for these technologies are decreasing, thus reducing the cost of electricity.

Analyzing more detailed data provided by the IRENA (International Renewable Energy Agency), in the period between 2010 and 2018, the average cost of electricity produced by PV (photovoltaic) panels went from 250 to 56 USD·MWh^{-1}, while from wind reduced from 75 to 48 USD·MWh^{-1}. Also, the lowest contracted energy records were 13.1 USD·MWh^{-1} for PV panels in Portugal and 20.5 USD·MWh^{-1} for wind in Brazil, both in the year 2019 [2].

1.1.2 Scalable Technology

The capital costs of electrolysis have been reduced ca. 60 % since 2010, resulting in a consequent decrease in the cost of hydrogen, from 10-15 to 4-6 USD·kg^{-1} [5]. According to a study carried out by the Hydrogen Council (Figure 3) the learning curve for both alkaline and PEM electrolysers is 9 % and 13 %, respectively. Therefore, it can be concluded that the capital costs of these technologies is expected to decrease in the upcoming years.



1. Installed base: assuming 50/50 split of electrolysers volume with 50-75% utilisation; assuming 115 kW for PV, 250 kW for buses and 300 kW for trucks; LCOE used for solar cost; batteries in MWh

Figure 3 - CAPEX evolution by total accumulated production (extracted from [5])

1.1.3 Benefits for the Power System

Most of the energy from renewable sources displays a time dependent behavior (i.e. wind, sunlight, etc.), being then named as variable renewable energy – VRE. The implementation of electrolysers allows for greater system flexibility as they can operate at different load percentages to compensate for fluctuations of VRE. Large amounts of energy produced when VRE is high cannot be stored, but green hydrogen produced with it, can. This enables the usage of this energy latter, when VRE levels are low.

1.1.4 Government Goals and Objectives

According to a study carried out by IRENA in 2020, over 120 countries have announced targets for zero-emissions of greenhouse gases (GHG). Among these is China, which is the largest emitter of GHG. China announced the goal of zero-emissions within 40 years [2]. This is also the country that in 2019 accounted for about 95 % of the total increase in global electricity production (total growth of 360 TWh in the world, 340 TWh in China) [4].

Figure 4 represents the shares of energy produced regionally, split by source, in 2019.

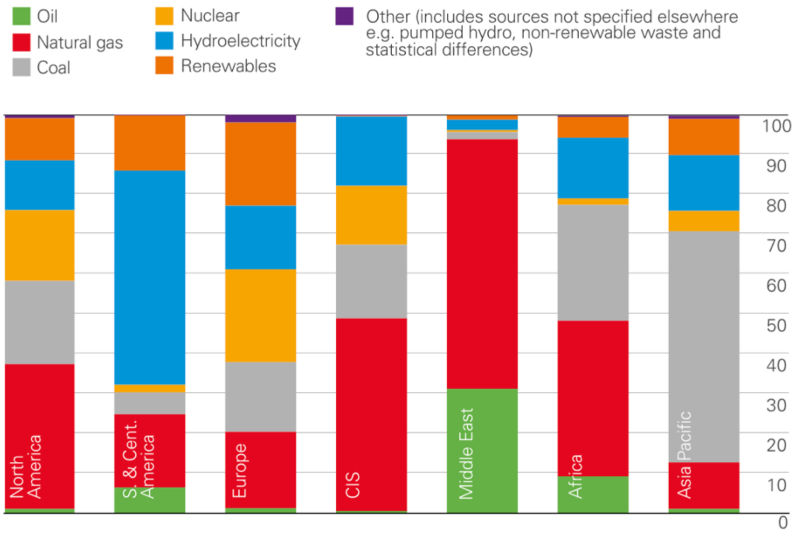


Figure 4 - Regionally produced energy quotas by energy source (extracted from [4])

The largest expression of Renewables is in Europe, followed by Central and South America, whilst Middle East and Asia appear as the largest emitters of GHG on energy production, relying mostly on non-renewable energy sources.

1.1.5 Diversified use of H_2

The annual production of H_2 is around 70 Mton, mostly being used in oil refineries and ammonia production. Recently a new business opportunity has arisen in the transport sector with fuel cells, and it is expected to reach 2.5 million units by 2030 [6].

Hydrogen can also be used as an energy carrier, given the possibility of storage and transportation for latter usage, wherever. Beyond that, green hydrogen can also be used as a feedstock for various chemical industries, helping to decarbonize other sectors and activities.

1.1.6 Interest of multiple stakeholders

Considering all the facts set out in previous points, there are multiple interested parties orbiting this technology, from public to private institutions. These “stakeholders” include energy service companies, steel manufacturers, chemical companies, port authorities, car, heavy-duty transportation and aircraft manufacturers, ship owners and airlines, and even at the government level there is a lot of interest on these technologies [2].

1.2 Presentation of the company

EFACEC is a Portuguese company established in 1905. It has been through a lot of changes ever since, but what is notable is the growth it has experimented. Nowadays, EFACEC’s revenue is roughly 75 % exports, from a total of 354M € with an EBITDA of 22M €. It has over 2500 employees, from which 87 % are In Portugal. The main business areas are the manufacturing of transformers (113 M€), energy applications (57 M€), electrical panels (60 M€), automation (50 M€) and electrical mobility (41 M€). The core company values are Reliability, Sustainability, Competence, Audacity and Humanism.

1.3 Contribution of the author to the work

The present work carried out by me comprehends five parts. In the first part, an introduction on the topic is provided. In the second part, I reviewed the state-of-the-art technology to be incorporated in the project. In the third part, which is the technical analysis of the project with all its units, I’ve used a software called SimulationX. This tool enabled me to mount all the process, gathering all the units that are necessary and testing them, both independently and together, through various simulations. In the fourth and fifth parts of the work, I’ve presented the simulation results along with a financial analysis of the project, with some market analysis, costs structure, revenues and finally the indicators from which conclusions can be drawn like the NPV - Net Present Value.

1.4 Organization of the dissertation

To achieve the final objective, the work was divided into several “sub objectives” that resulted in the established goal.

Chapter 1 provides an introductory overview on the energy production and hydrogen markets.

Chapter 2 frames the work developed and presents the state-of-the-art.

Chapter 3 addresses the technical analysis of the project, supported by the simulation software “SimulationX” by ESI Group. This Chapter addresses each of the project’s components, moving on to a broader overview of the whole process by the end.

Chapter 4 contains the simulation results as well as a financial analysis of the project. The financial analysis covers Cost Analysis, Revenues and finally some KPI (Key Point Indicators) like the net present value.

Chapter 5 presents the conclusions drawn from both technical and financial analysis, to reach the proposed objective – to determine the viability of the Project.

2 Context and State of the art

This chapter presents the different equipment to include in the project, contemplating the most recent R&D advances in the area. Both advantages and disadvantages for each equipment will be listed. The main thread in this section will follow the processual chain, starting from the water input to the system until the H_2 storage and system output.

2.1 Water Treatment

Electrolysers are very sensitive to water contaminants such as ions and particles because they can hinder the ionic permeation through the ion exchange membrane, either cation exchange (PEM electrolyser) or anion exchange (AEM electrolyser). Ions, especially multivalent ions and heavy ions, exchange strongly at the membrane hindering the balancing current of protons (PEM electrolysis) or hydroxyl ions (AEM electrolysers), which permeate the membrane based on an ion-exchange mechanism. Additionally, particles can cause the membrane fouling and affect the membranes capacity to permeate protons [7]. The water fed into the electrolyser must be controlled once it can carry water soluble components like K^+ and Na^+. Other substances can be diluted in water as well, such as iron, manganese and hydrogen sulfide, that can greatly hinder the process efficiency [8]. One method to insert this type of control in the process is to monitor the water conductivity. The more ions it bears, the higher value of conductivity comes in the output. One way to keep the water conductivity low is to properly degas the water during the deionization process. A water treatment system is set before the electrolyser inlet. Many methods can be used to control water conductivity, but different methodologies lead to different results. The specific requirements of water purity also depend on the electrolyser technology. The water fed into an alkaline electrolyser does not need to be so rigorously pure as it would in a PEM electrolyser [9], as it will be further discussed on the next section. The minimum standard for water for PEM electrolysis is deionized water. The conductivity of this water is between $0.1 – 10\ \mu S \cdot cm^{-1}$ [10]. This can be achieved by using an ion exchange resin. Typically, these units are composed of a cation bed, an anion bed and a mixed bed, connected in series. The mixed bed, also known as polisher, is composed of both cation and anion resins, and drastically improve the overall unit efficiency [11]. The cation bed is used to remove positively charged ions like calcium, magnesium and sodium, while the anion bed removes negatively charged ions such as sulfate and chloride [11]. This is especially important because in PEM electrolysis, chloride will foul PGM catalysts and cations reduce the membrane's proton conductivity [9].

2.2 Electrolysis

High quality hydrogen (purity of 99.999 %) can be produced through water electrolysis, unlike other methods such as SMR, where the hydrogen stream is contaminated with carbon derived species such as carbon monoxide and other pollutants [7]. In this equipment, water is split into hydrogen and oxygen, following the reaction represented in Eq. (1):

$$\mathrm{H_2O} \rightarrow \mathrm{H_2} + \frac{1}{2}\mathrm{O_2} \qquad (1)$$

As this is an endothermic reaction, it is needed 237.2kJ·mol^{-1} that corresponds to the electric energy input and 48.6 kJ·mol^{-1} to the heat, necessary for the reaction to occur [7].

Throughout the past, the high cost of electricity has called into question the economic feasibility of hydrogen production through this process [12]. However, with the recent growth of renewable energy production such as wind and PV, the paradigm is about to change [13]. Hydrogen produced through electrolysis with renewable electricity assumes several functionalities, from an energy vector, to serve as feedstock for other chemical applications, or even to act as fuel for transportation purposes. This helps to bridge the intermittency of renewable energy availability [14, 15].

2.2.1 Alkaline Electrolyser

Ever since the discovery of the electrolysis phenomenon by Trooostwijk and Diedmann in 1789 [16], alkaline electrolysis has been extensively developed. Electrolyser units have reached a mature stage for the production of hydrogen up to the megawatt range, being the most commercially extensive electrolysis technology worldwide [17].

This technology is characterized by having two electrodes immersed in an alkaline electrolytic liquid consisting of a caustic potassium solution with a KOH concentration of around 20 – 30% [7] (Figure 5).

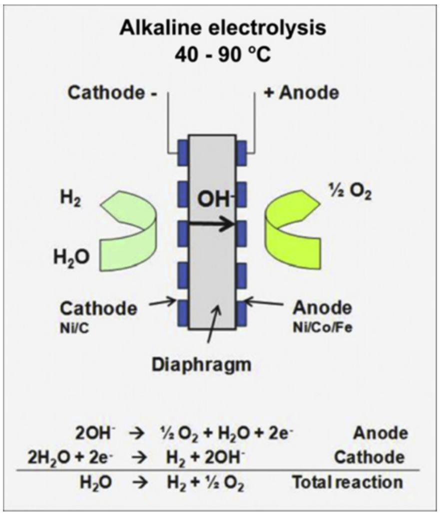


Figure 5 - Alkaline electrolyser operation scheme (extracted from [7])

The two electrodes are separated by a diaphragm that has the important role of keeping the two gaseous products apart. This is important primarily for the sake of efficiency, but also for safety reasons. The diaphragm must be permeable to OH^- ions and H_2O molecules [7]. The state-of-the-art values for the specifications of this technology are listed in Table 1.

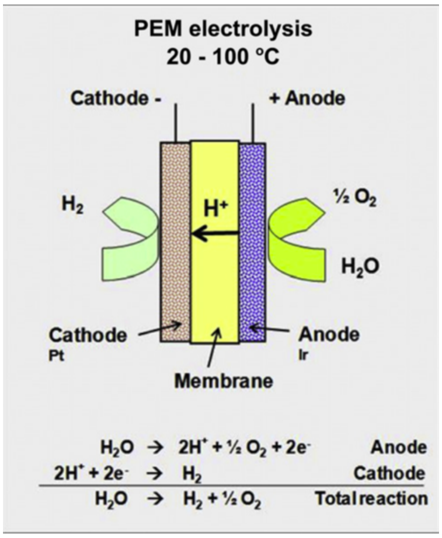
Table 1 - State-of-the-art specifications for an Alkaline Electrolyser [18]

Specifications	Alkaline Electrolysis
Cell Temperature (ºC)	60 — 80
Cell Pressure (bar)	< 30
Current Density (mA cm^{-2})	0.2 — 0.4
Cell Voltage (V)	1.8 — 2.4
Power Density (mW cm^{-2})	< 1
Voltage efficiency HHV (%)	62 — 82
Specific energy consumption: stack (kW h Nm^{-3})	4.2 — 5.9
Specific energy consumption: system (kW h Nm^{-3})	4.5 — 7.0
Lower partial load range (%)	20 — 40
Cell area (m^2)	> 4
H_2 production rate: stack-system (Nm3 h^{-1})	< 760
Stack Lifetime (h)	< 90,000
System lifetime (years)	20 — 30
Degradation rate (µV h^{-1})	< 3

However, there are three main problems associated with the use of this technology – low partial load range, limited current density and low operating pressure [7]. The diaphragm cannot completely prevent the segregation of gases that diffuse thorough it. Diffusion of oxygen into the cathode chamber reduces the efficiency of the process, as it will re-form water molecules when in contact with hydrogen. On the other hand, the diffusion of hydrogen to the anode side can have more dangerous consequences. In addition to the decrease of the overall electrolyser efficiency, the lower explosion limit in this situation is >4% mol H_2 in O_2 [19]. The second problem is the fact that the maximum achievable current density value is low, due to the high ohmic losses through the electrolytic liquid and the diaphragm. Finally, the impossibility of operating at higher pressures, also due to the electrolytic liquid, makes for a very bulky design and adds additional costs for latter pressurizing the hydrogen stream [7].

2.2.2 PEM Electrolyser

Around 1960's, General Electric developed the first electrolyser based on a solid polymer electrolyte [20]. This concept was devised by Grubb [21, 22], where a solid polystyrene sulfonate membrane was used as the electrolyte. This process is referred to as Proton Exchange Membrane or Polymer Electrolyte Membrane, both having the acronym PEM. The polymer electrolyte membrane (PEM) is responsible for providing a very large proton conductivity, low gas diffusion, the ability to operate at high pressures and a compact format. These capabilities solve most of the issues raised by the Alkaline Electrolysis. One of the reasons why this is possible is due to the fact that the membrane's thickness is normally between 20 – 300 μm [7]. A schematic of the operation of such an electrolyser is presented in Figure 6, as well as the state-of-the-art values for this technology (Table 2).



$$\begin{array}{lcll} H_2O & \rightarrow & 2H^+ + \tfrac{1}{2} O_2 + 2e^- & \text{Anode} \\ 2H^+ + 2e^- & \rightarrow & H_2 & \text{Cathode} \\ \hline H_2O & \rightarrow & H_2 + \tfrac{1}{2} O_2 & \text{Total reaction} \end{array}$$

Figure 6 - PEM. electrolyser operation scheme (extracted from [7])

Table 2 - State-of-the-art specifications for a PEM Electrolyser [7]

Specifications	PEM Electrolysis
Cell Temperature (ºC)	5 — 80
Cell Pressure (bar)	> 30
Current Density (mA cm^{-2})	0.6 — 2.0
Cell Voltage (V)	1.8 — 2.2
Power Density (mW cm^{-2})	< 4.4
Voltage efficiency HHV (%)	67 — 82
Specific energy consumption: stack (kW h Nm^{-3})	4.2 — 5.6
Specific energy consumption: system (kW h Nm^{-3})	4.5 — 7.5
Lower partial load range (%)	10 — 0
Cell area (m^2)	< 0.03
H_2 production rate: stack-system (Nm3 h^{-1})	< 10
Stack Lifetime (h)	< 20,000
System lifetime (years)	10 — 20
Degradation rate (μV h^{-1})	< 14

Exploring in more detail the advantages listed above, PEM electrolysers can operate at much higher current densities, capable of reaching values above 2 A·cm^{-2}, hence reducing the operation costs and potentially the overall cost of the process. The ohmic losses limit the maximum achievable current densities, so by having a very thin membrane capable of providing a very high proton conductivity (0.10 ± 0.02 S·cm^{-1}) [23], higher current densities can be achieved. The low gaseous diffusion rate of the membrane has several benefits as well. First, the efficiency of the process tends to be higher, as does the purity of the hydrogen current. This factor also allows the electrolyser to operate at a wider power range, which is also an important economical feature itself. This happens because the proton permeation across the membrane responds rapidly to the input power, unlike in liquid electrolytes. In this case there is not a problem working at low load, because the hydrogen concentration in the anode side will not increase (like it would in the alkaline electrolyser), thus not escalating to hazardous scenarios. PEM electrolysers cover practically the entire nominal power range spectre (10-100% load) [24]. Solid electrolytes allow for a more compact system design with structural strength properties where it is possible to operate at high pressures (which can vary through the electrolyte itself) [25]. Some commercial applications claim to have already reached operating pressures up to 350 bar [26]. The operation at high pressure of an electrolyser brings the advantage that the hydrogen stream is already pressurized in the outlet (a process that can be called electrochemical compression) [27], thus less energy is required to further compress it and store it. In addition, it also reduces the volume of the gas phase at the electrodes favouring the extraction of the gaseous products, which follows Fick's Law [28]. In a differential pressure configuration, only the cathode is under pressure, this can eliminate the hazards related to handling pressurized oxygen, such as the risk of autoignition of Ti in oxygen [29].

Regarding the negative aspects of this technology, there are some problems related to the operation at high pressures, such as the phenomenon of cross diffusion that increases with the operating pressure increase [30, 31]. Pressures above 100 bar require the use of thicker membranes and recombination of gases to keep critical concentrations, especially H_2 in O_2 below safety limits. A lower gas permeability value across the membrane can be obtained by incorporating several different filters into the membranes constituent material [32], but this usually results in a material with a lower proton conductivity. The acid corrosive environment provided by the PEM requires the use of materials with certain characteristics. The choice of these materials must consider the capacity of resisting this harsh corrosive environment and withstand a high applied voltage (~2V), especially at high current densities [7]. Corrosion resistance should be a characteristic not only for materials composing the catalyst, but also to the current distributors and separator plates. Only a few materials match these criteria and all of them are rare and expensive. These are noble catalysts based on PGM (Platinum Group Metals – e.g. Pt, Ir and Ru), current distributors and separator plates based on titanium [7]. This is one of the major disadvantages of this technology, once the need to use this scarce and expensive materials has a great impact on the project capital costs.

2.3 Hydrogen Purification

Depending on the end-use of the hydrogen, different levels of purity are required. For example, for fuel cell vehicles, high-purity standards are required. The presence of contaminants is mostly affected by the production pathway. From the electrolysis of water, there are three main pollutants: Nitrogen, Oxygen and Water [8]. In fact, there are guidelines for the commercialization of hydrogen and can be consulted, such as ISO 14687:2019 standard [33].

The work of Yorick Ligen et al. provides a very rich insight on this technology and goes as follows. The experimental work conducted, consisted in a commercial 50 kW alkaline electrolyser, and were used several analytical techniques such as gas chromatography and mass spectrometry - this experimental work stretches out from the project scope, but a scale-up analysis can be done.

To purify the hydrogen stream from this commercial unit, it is necessary to know which are the contaminants and how much is their presence in the product stream:

- Nitrogen – this gas is often used to purge electrolysers during maintenance, shut down and/or start up sequences. Although it is an inert, it dilutes the concentration of hydrogen. Typically, there is no need to add any special unit to remove this gas. Often it is just needed to vent out the initial production to get to the ISO 14687:2019 levels. If nitrogen presence is further noticed in continuous production, that is a different scenario. In that case, it is very likely that nitrogen is dissolved in the water stream fed to the electrolyser. The solution for that would be simply to make sure that water is being properly degassed prior or during the deionization process [8].
- Oxygen – The maximum amount of oxygen that can be fed to a fuel cell in the hydrogen stream is 500 ppm. The most common way of removing the oxygen is using a catalytic recombination process as indicated in Eq. (2):

  $$\mathrm{O_2} + 2\mathrm{H_2} \underset{\mathrm{Cat.}}{\longrightarrow} 2\mathrm{H_2O} \tag{2}$$

  As this is an exothermic reaction and water is produced, this step is usually followed by a condensation drying step.

- Water – The presence of water in the hydrogen stream can represent more problems than one might think. It can, for example, form ice and affect control components. Therefore, a 5 ppm limit ensures that water remains gaseous even in high pressures and low ambient temperatures. However, the content of water bearable in a PEM fuel cell is 500 ppm, as long as it does not affect any internal flows [34]. The stream of hydrogen on the alkaline electrolyser outlet is saturated with water at the operation temperature, thus most of the water can be removed just by simply applying a cooling process. Freezing temperatures should still be avoided because of the formation of ice. A dew point of 5 °C at 10 and 40 bar corresponds, respectively, to 1000 and 200 ppm of water [8], so it is still needed to dry beyond that in order to reach 5 ppm. For this, a VPSA (Vacuum Pressure Swing Adsorption) unit is normally the technology considered [35-37].

Table 3 shows the specifications of the electrolyser used in the work of Yorick Ligen et al. and Table 4 the specifications of the VPSA unit to be coupled with this type of electrolyser.

Table 3 - Electrolyser specifications [8]

Parameter	Value
Nominal Power (DC)	50 kW (2 x 25 kW stack)
Nominal production rate at 300 mA/cm^2	850 g H_2/h
Cells per stack	115
Geometric electrode surface area	370 cm^2
Electrode gap	5.5 mm
Current density	160 – 320 mA/cm^2
Electrolyte	30 wt% KOH (ca. 60 L)
Inertization and pressurization media	Nitrogen 99.999%
Temperature of operation	Stack inlet: 52.5 °C (regulated) Stack outlet: 60 – 75 °C 10 bar
Operating pressure	10 bar
Gas cooling	5 °C chilled water with plate heat exchangers

Table 4 - VPSA specifications [8]

Parameter	Value
Column Volume	3.8 L per column, height 60 cm, diameter 9 cm
Empty column volume	2.6 L
Desiccant type	Molecular sieve 4A, beads 8 – 12 mesh
Desiccant loading	2.77 kg per column
Operating pressure	35 – 38 bar, regeneration at 0.1 mbar
Vacuum pump	Edwards nXDS 15i
Purge flow limiter	PEEKsil capillarity tubing 50 cm, 25 um internal diameter
Cycle Duration	10 min

The alkaline electrolyser used. In the experimental procedure was based on commercial stacks from McPhy, model McLyzer 10-10, although some parameters were altered for better performance [38]. A standard start-up and shut-down procedure were carried out using nitrogen, to recreate an inert environment that simulates long stand-by periods, before current was applied. Three units were used to remove all pollutants: a scrubber to remove KOH, a deoxygenation reactor where the catalytic recombination of oxygen occurs and after the outlet gas is cooled and part of the water is removed with a filter, the hydrogen is further dried in a VPSA unit working at 40 bar [8].

The VPSA was designed to take advantage of the compression step that occurs before this unit (10 bar) and the final storage pressure (200 bar in this experiment case). Figure 7 provides a simplified scheme of the operation process.

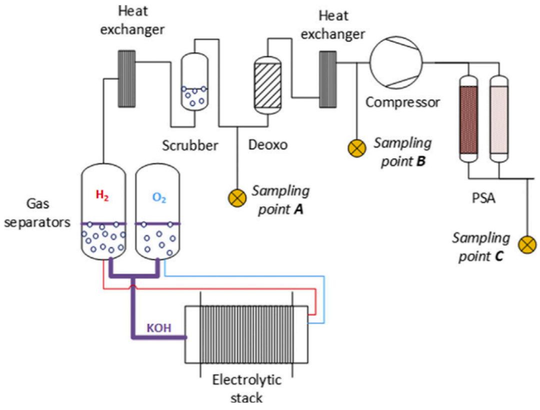


Figure 7 - Simplified flowsheet of purification and drying steps (extracted from [8])

To sum up, the nitrogen was accomplished purging the initial production. In this experimental work, nitrogen levels were kept under ISO 14687:2019 after 100 min of operation time. This also confirms the hypothesis that the presence of this component is due to the stand-by periods (maintenance and start-up/shut-down) where nitrogen is used. With the deoxygenation reactor, levels of oxygen were kept between 1 – 4 ppm, but the exothermic nature of the catalytic recombination of hydrogen into water makes it indispensable to add a cooling system after it, so part of the water is removed from the stream. Finally, the most energy intensive step, the drying in the VPSA. A hydrogen recovery performance of 98.4% with a water content below 0.1 ppm and an anergy consumption of 0.5 kWh per kilogram of hydrogen produced [8].

2.4 Compression

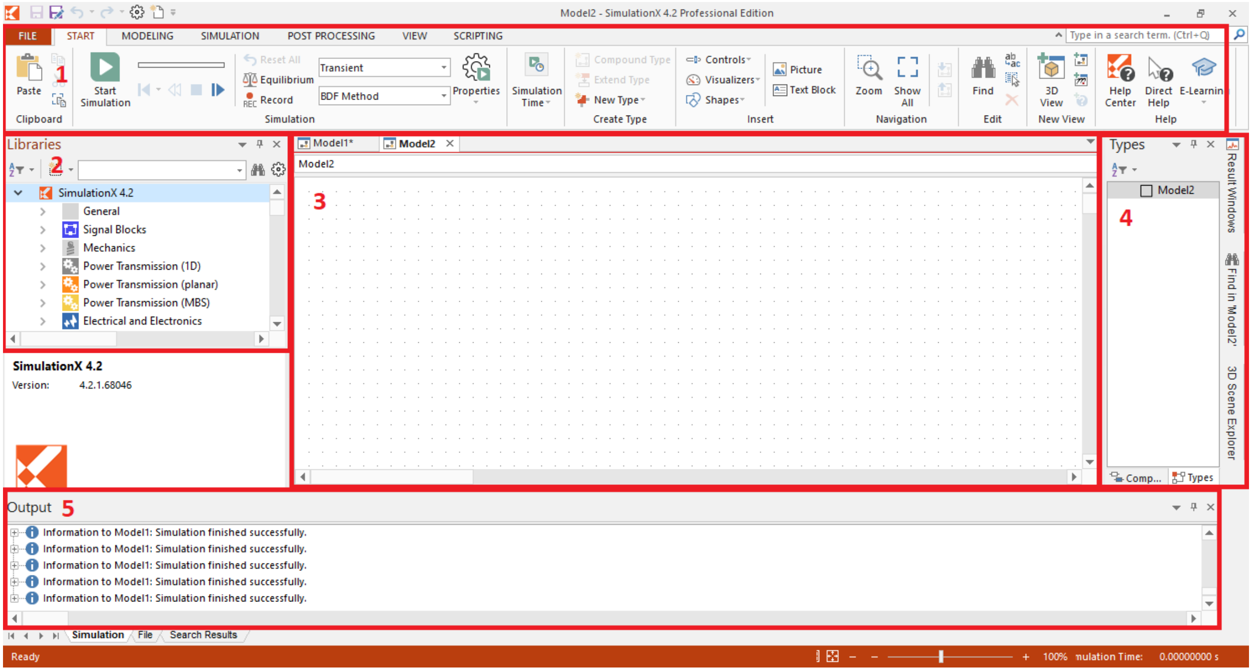
Hydrogen has the lowest volumetric energy density between the most universally used fuels at atmospheric pressure – 0.01079 $MJ \cdot L^{-1}$ [39], which is much smaller than the one of petrol – 34 $MJ \cdot L^{-1}$ [40]. Therefore, compression is a fundamental step to add to the system to overcome this issue. There are two main groups of compressors characterized by their *modus operandi*. Mechanical compressors are the most used today and basically, what they do is a simple conversion of mechanical energy into gas energy. The typology for this is referred as “positive displacement”, which means that these work by reducing the confined volume in which hydrogen is contained with a piston. In other words, H_2 is squeezed into a smaller volume mechanically, resulting in an increase of the number of collisions between the molecules and the walls [41] resulting in an increase of the gas pressure. Non-mechanical compressors are the alternative for the old-fashioned mechanical compressors. This more recent technology seems to be more efficient once the need for great amounts of energy is in order to compress enough gas mechanically [42]. For this project, the compressor stage is based on mechanical compressors. Since the purity of hydrogen is to be preserved, the best way to do so is to use diaphragm compressors. In these units, there is no direct contact between the piston and the gaseous products. The piston transmits its energy into a liquid that itself will push a metallic layer (diaphragm) that isolates hydrogen. The American company PDC Machines is the leader in manufacturing this type of technology as their compressors can operate at a discharge pressure of 517 bar with flow rates from 50 to 280 $Nm^3 \cdot h^{-1}$ [43].

2.5 Storage

Hydrogen storage and transportation are now being under fast development. These processes play an important role in hydrogen economy. The goal is to be safe and efficient, so it can be used anywhere, anytime. Pure hydrogen has low volumetric energy density but high gravimetric energy density [44]. There are three methods used to store hydrogen. Physical storage as compressed gas, physical storage as cryogenic liquid and solid state storage methods [45]. The most common ways of storage for this substance are as compressed gas and as cryogenic liquid. Storing hydrogen as compressed gas enables the pressurization of the stream up to 700 bar in gas cylinders. This kind of pressure is more common for small transportation like in Fuel Cell Vehicles (FCV). Larger storage units or transportation use hydrogen compressed at 350 bar. Compressed gas storage containers are made of steel, aluminium and carbon fibber reinforced plastic composite materials [46]. There are also some studies being conducted, to assess the possibility of storing hydrogen in underground salt caves [47]. Storing hydrogen as a liquid has the advantage that its density is greater than the one of compressed gas, storing more energy per volume unit [44]. The downside to this technology is the fact that hydrogen must be stored at -253 °C and the boiling point is very low. Consequently, special vessels with insulation systems are necessary in order to preserve the hydrogen [46, 47].

2.6 Simulation Software

Technical systems are often very complex. This project's plant is no different, with a vast and diversified number of equipment that must be designed separately but still must work together. Hence, it is necessary to find a space where one can assemble everything together. SimulationX by ESI Group is a software that can be used for modelling, simulation and analysing technical systems. The software comes with a series of built-in libraries, but it is also possible to create new components, assemble compounds, or even create new sets of libraries from scratch. The programming language it uses is Modelica, which is a very standard open-source computing object-oriented language. The benefits of using SimulationX are to shorten development time by using models to quickly test the effects of various design or process changes; saving time and money by not needing to actually build real prototypes; develop and test control software and hardware with a virtual plant before the system is built; carry out extensive simulation-based experiments to identify potential design problems early on; possibility to create a digital twin and run it in parallel to the real system to monitor the conditions and faults that might happen [48]. Figure 8 shows the software main screen edited in a way the most important features are highlighted.



SimulationX 4.2
Version: 4.2.1.68046

```
Information to Model1: Simulation finished successfully.
Information to Model1: Simulation finished successfully.
Information to Model1: Simulation finished successfully.
Information to Model1: Simulation finished successfully.
Information to Model1: Simulation finished successfully.
```

Figure 8 - SimulationX software (edited screenshot)

As it can be observed from Figure 8, even though SimulationX offers a great number of functionalities, its output is very user friendly. From Figure 8, sector 1 contains a tool bar, where one can navigate through the software multi functionalities. It is also the place where the start button is for the simulation, as well as the panel to define the system properties and timespan. Sector 2 is where all the built-in libraries can be found. There, one can also create new classes like models, connectors, records, blocks, etc. the new classes will also appear on this section. Sector 3 is the canvas. This is where the blocks are created, compounds are assembled through block connections and serve as the base for the model simulation. Sector 4 is a quick menu finder, where one can select which component to analyse and choose any result from the result window. Finally, sector 5 is the output screen, where information on the simulation is presented. It always provides feedback whether the simulation has run successfully or not. In case there was something wrong, this screen will point out the type of error and the root cause, so it is easier to rectify.

3 Technical Analysis

The technical analysis covers the modelling of the electrolyser as well as the assembly and simulation of the whole plant. It starts with a set of equations that define the electrolysis process and moves on to the implementation of these equations on the simulation model.

3.1 Electrolyser Model

Contrary to the modelling of the PEM Fuel Cell that started around 1990 [49], PEM electrolysis is quite recent, with the first reported models appearing around 2002 [50]. In the first phase of PEM electrolysis modelling, Faraday's law was widely used to determine the steady state approximation of the cell polarisation curve [50-53]. This one-dimensional view of steady state approximation greatly limits the ability of the model to predict scenarios required for control system optimisation, limiting the ability to examine integration in an intermittent system. With the progression of models, in 2005 the first dynamic model of PEM electrolysis appeared [54]. More recently, the first multidimensional models began to appear with the aim of examining individual components of the electrolyser, from the separator plates [55, 56] to the electrical resistance of the stack [57]. However, these only served to model components individually. Despite all the progress made in this field of research, the modelling of PEM electrolysis still lags far behind the modelling of PEM fuel cells. Alkaline electrolysis on the other hand, is a mature knowledge at the moment.

Even though the two different methods have different cell constitution and materials, the result is pretty much the same. Water is split into hydrogen and oxygen. The energy needed for this to happen is given by the change in enthalpy:

$$\Delta H = \Delta G + T \cdot \Delta S \; [\mathrm{J \cdot mol^{-1}}] \tag{3}$$

the amount of energy in the form of electricity that has to be supplied in order for the reaction to occur is given by the change in Gibbs free energy (ΔG) that under standard conditions is equal to ΔG = 237.23 kJ·mol-1 [58]. Hence, the theoretical minimum potential needed is:

$$E_{\mathrm{rev}} = \frac{\Delta G^0}{z \cdot F} = \frac{273.23 \cdot 10^3}{2 \cdot 96485} = 1.23 \text{ V} \tag{4}$$

in which *z* is the number of electrons transferred and *F* is the Faraday constant (*F* = 96 485 C·mol^{-1}). U_{rev} is the reversible potential, and it corresponds to the lower heating value (LHV) of hydrogen. Nonetheless, for the reaction to actually happen the energy needed to overcome is actually the hydrogen higher heating value (HHV) which is the change in enthalpy ΔH^0 = 285.5 kJ·mol^{-1} [58].

$$E^0 = \frac{\Delta H^0}{z \cdot F} = \frac{285.85 \cdot 10^3}{2 \cdot 96485} = 1.48\ \mathrm{V} \tag{5}$$

This is the thermoneutral voltage, which corresponds to a cell operating at the minimum voltage, thus not producing or consuming heat. This would correspond to a hypothetical situation where there would not be losses due to resistance or other causes, but it is not like this. To model a cell, it is necessary to figure out the operation voltage, E_{cell}:

$$E_{\mathrm{cell}} = E_{\mathrm{therm}} + \eta_{\mathrm{act}} + \eta_{\mathrm{ohmic}}\ [\mathrm{V}] \tag{6}$$

where E_{therm} is the thermodynamic potential, η_{act} is the activation overpotential and η_{ohmic} is the cell's ohmic losses.

$$E_{\mathrm{therm}} = E_{\mathrm{rev}} + \frac{R \cdot T}{z \cdot F} \ln\left(\frac{P_{\mathrm{H_2}} P_{\mathrm{O_2}}^{\frac{1}{2}}}{P_{\mathrm{H_2O}}}\right) [\mathrm{V}] \tag{7}$$

E_{rev} is the reversible potential, as in Eq. (4), *R* is the universal gas constant (*R* = 8.3145 J·mol^{-1}K^{-1}) and P_i is the partial pressure. For water this is equivalent to 1 and for gases (P_i / P^0) with P^0 = 1 bar.

$$E_{\mathrm{rev}} = \frac{\Delta G(T)}{z \cdot F}\ [\mathrm{V}] \tag{8}$$

For *T* = 298 K, E_{rev} is 1.23 V but as in most commercial applications the reaction does not happen at that temperature, the model needs to rely on an empirical relation between the reversible potential and the operation temperature [59]:

$$E_{\mathrm{rev}}(T) = 1.5184 - 1.5421 \cdot 10^{-3} T + 9.523 \cdot 10^{-5} T \ln T + 9.84 \cdot 10^{-8} T^2\ [\mathrm{V}] \tag{9}$$

up until this point, a relation between E_{therm} with operating pressure and temperature is set. Moving on to the activation overpotentials, the voltage applied for water splitting must consider more than just thermodynamics. The kinetics of the oxygen and hydrogen evolution reactions (OER and HER, respectively) are limited and dependent on the temperature, pressure and catalysts used. The relation between the theoretical current, *i*, and the overpotentials is given by the Butler-Volmer equation that can be adapted for both half reactions of each electrode:

$$i = i_0 \left[\exp\left(\frac{\alpha \cdot z \cdot F \cdot \eta_{act}}{R \cdot T}\right) - \exp\left(-\frac{(1-\alpha) \cdot z \cdot F \cdot \eta_{act}}{R \cdot T}\right)\right] \; [\mathrm{A \cdot cm^{-2}}] \tag{10}$$

i_0 is the exchange current density $[\mathrm{A \cdot cm^{-2}}]$, α is a dimensionless transfer coefficient and *z* the number of transferred electrons. The equation can be rearranged for both anode and cathode:

$$\eta_{\mathrm{act,a}} = \frac{R \cdot T}{\alpha_a \cdot z \cdot F} \ln\left(\frac{i}{i_{0,\mathrm{a}}}\right) \; [\mathrm{V}] \tag{11}$$

$$\eta_{\mathrm{act,c}} = -\frac{R \cdot T}{\alpha_c \cdot z \cdot F} \ln\left(\frac{i}{i_{0,\mathrm{c}}}\right) \; [\mathrm{V}] \tag{12}$$

both α_a and α_c can be considered approximately equal to 0.5. This is, however, a simplification; strictly this is only true for electrochemical reactions involving the exchange of just 1 electron in a reaction mechanism involving a single reaction step. The values for the current exchange density can be approximated using an Arrhenius relation, with i_o^{ref} taken from the literature [7], as follows:

$$i_0 = i_0^{\mathrm{ref}} \cdot \exp\left[\frac{E_{\mathrm{act}}}{R}\left(\frac{1}{T^{\mathrm{ref}}} - \frac{1}{T}\right)\right] \; [\mathrm{A \cdot cm^{-2}}] \tag{13}$$

with this, a relation is made between the activation overpotentials and the operating current density and temperature. Lastly, the ohmic overpotential is the result of ohmic resistance in the cell. This resistance is mostly accounted for the conductivity in the PEM, with a small contribution of electrical resistance that can be neglected in this case. Most literature uses a semi-empirical equation [49] to calculate the conductivity in the membrane:

$$\sigma_{\mathrm{m}} = (0.005139\lambda - 0.00362)\exp\left[1268\left(\frac{1}{303} - \frac{1}{T_{cell}}\right)\right] \; [\mathrm{S \cdot cm^{-1}}] \tag{14}$$

where λ is the water content of the membrane and can be calculated through the following equation:

$$\lambda = 0.043 + 17.81a - 39.85a^2 + 36.0a^3 \tag{15}$$

where a is the water activity, which in the case of water electrolysis is equal to 1. Hence it is possible to get to a value of σ_{m}, so with a value for the membrane thickness, t_{m} is then possible to get to its conductivity.

$$R_{\mathrm{m}} = \frac{t_{\mathrm{m}}}{\sigma_{\mathrm{m}} \cdot A_{\mathrm{cell}}} \; [\Omega] \tag{16}$$

Ideally the model should include the resistance from bipolar plates and current distributors as well, but in this case, the only resistance accounted is from the membrane itself, which accounts for the most part of the ohmic resistance.

$$\eta_{\mathrm{ohmic}} = R_{\mathrm{m}} \cdot i \cdot A_{\mathrm{cell}} \ [\mathrm{V}] \tag{15}$$

With this last part of Eq. (6), η_{ohmic}, correlated with the current density, it is finally possible to get to the polarization curve, where the voltage is presented as a function of the current density, hence the two major ingredients to solve out the power of the electrolyser. For the next part, it is essential to figure out the stream of hydrogen. Faraday's law can be applied to calculate the compositions of the product flows as follows:

$$Q_{\mathrm{H_{2,c}}} = \frac{\mathrm{I}}{2 \cdot F} \cdot \eta_{\mathrm{F}} \ [\mathrm{mol \cdot s^{-1}}] \tag{16}$$

$$Q_{\mathrm{O_{2,a}}} = \frac{\mathrm{I}}{4 \cdot F} \cdot \eta_{\mathrm{F}} \ [\mathrm{mol \cdot s^{-1}}] \tag{17}$$

$$Q_{\mathrm{H_{2,a}}} = \frac{\mathrm{I}}{2 \cdot F} \cdot (1 - \eta_{\mathrm{F}}) \ [\mathrm{mol \cdot s^{-1}}] \tag{18}$$

$$Q_{\mathrm{O_{2,c}}} = \frac{\mathrm{I}}{4 \cdot F} \cdot (1 - \eta_{\mathrm{F}}) \ [\mathrm{mol \cdot s^{-1}}] \tag{19}$$

Most literature considers Faraday's efficiency, η_{F}, to be 0.99 [7]. In this case, it was not possible to incorporate multi-composition product flows, so the model is working on pure hydrogen and oxygen streams, although it is not real as stated in section 2.3 of this document. As the products form in water, it is expected that both the hydrogen and oxygen streams are saturated with water as well.

With the outlet streams solved out, it is necessary to figure out the amount of water to feed the electrolyser. The rationale for this starts with the reaction stoichiometry. Firstly, it is determined the number of hydrogen mols in 1 kg.

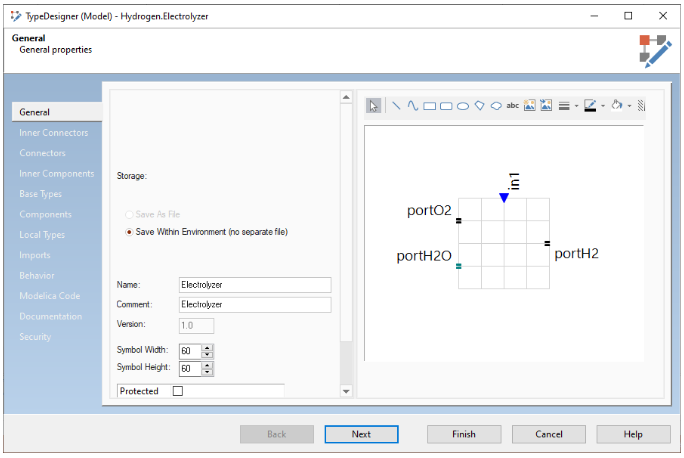
$$n_{\mathrm{H_2}} = \frac{1000}{M_{\mathrm{H_2}}} \ [\mathrm{mol}] \tag{20}$$

Where $M_{\mathrm{H_2}}$ is 2 g·mol^{-1}, which makes for 500 mol of hydrogen per kilogram. Then, all that is needed to do, is to multiply that number of mols with water's molar mass, once the reactions stoichiometry is 1 to 1.

$$m_{\mathrm{H_2O}} = n_{\mathrm{H_2}} \cdot M_{\mathrm{H_2O}} \ [\mathrm{g}] \tag{21}$$

As $M_{\mathrm{H_2O}}$ is 18 g·mol^{-1}, the value for the mass of water in this case is 9000 g, or 9 kg of water per hydrogen kilogram.

With all these equations, a mathematical model could be created on SimulationX. Under the modeling tab, “New Type > Model”, a new window opens (TypeDesigner) with every aspect that needs to be parameterized (Figure 9).

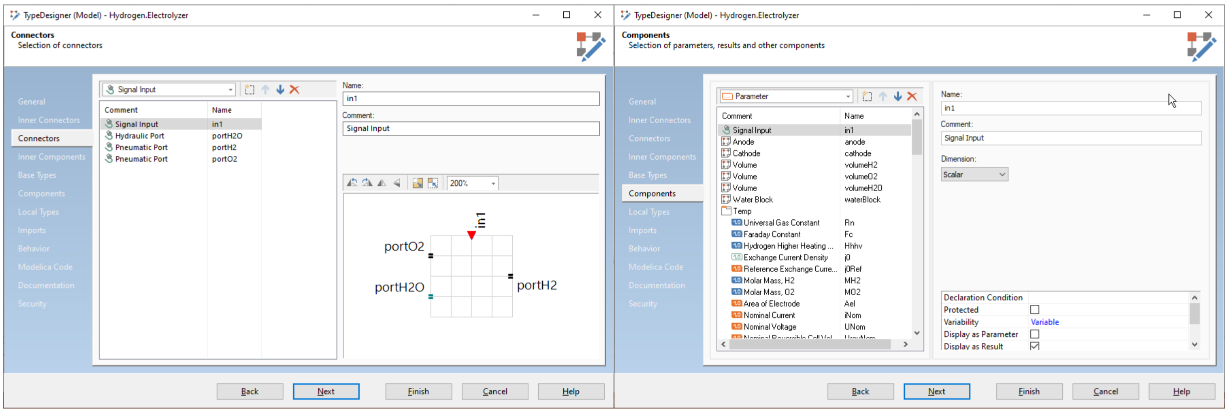


Storage:
○ Save As File
● Save Within Environment (no separate file)

Name: Electrolyzer
Comment: Electrolyzer
Version: 1.0
Symbol Width: 60
Symbol Height: 60
Protected ☐

Figure 9 - TypeDesigner

“General” (properties) is where one can define the model’s name and create a symbol that represents that block. “Inner Connectors” contains all the binding of inner connectors. All electrolyser constituents are here: anode, cathode, all 3 volume blocks, one for each substance (water, hydrogen and oxygen). All these inner connectors must have compatible ports so they can be connected. For example, for the water to enter the electrolyser, the water volume block must have 2 hydraulic ports, one to its source (inlet) and the other to feed the electrolyser (outlet). On the other hand, the electrolyser, on its anode, must have 1 pneumatic port for the oxygen outlet, as well as a hydraulic port for water inlet. All these ports can be defined in the “Connectors” tab. Inside “Inner Components” tab, all connectors, ports and connections can be monitored along with all physical properties (e.g. absolute pressure and temperature on the cathode). Under “components” is where one can create a new component (functional block, parameter, variable, etc.) to be part of the model.



TypeDesigner (Model) - Hydrogen.Electrolyzer

Connectors
Selection of connectors

Comment	Name
Signal Input	in1
Hydraulic Port	portH2O
Pneumatic Port	portH2
Pneumatic Port	portO2

Name: in1
Comment: Signal Input

TypeDesigner (Model) - Hydrogen.Electrolyzer

Components
Selection of parameters, results and other components

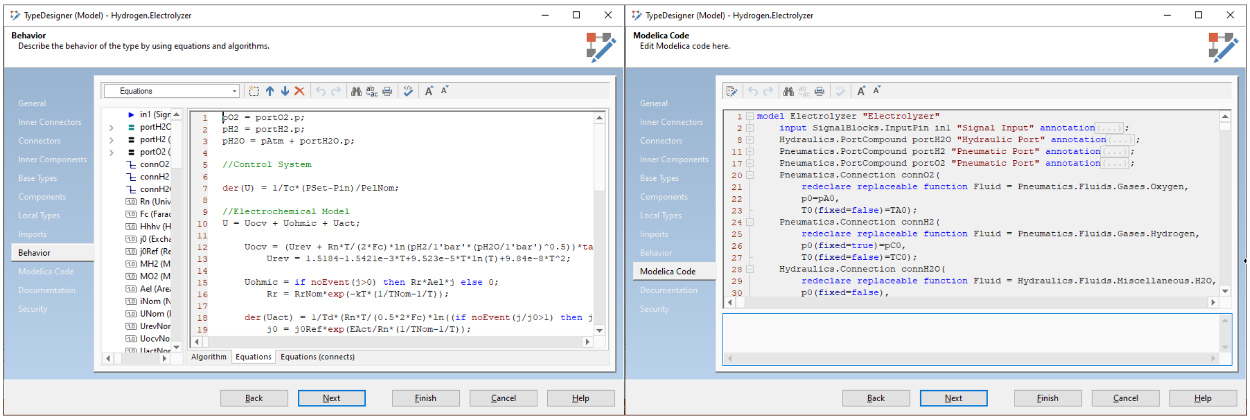
Comment	Name
Signal Input	in1
Anode	anode
Cathode	cathode
Volume	volumeH2
Volume	volumeO2
Volume	volumeH2O
Water Block	waterBlock
Temp	
Universal Gas Constant	Rn
Faraday Constant	Fc
Hydrogen Higher Heating ...	Hhhv
Exchange Current Density	j0
Reference Exchange Curre...	j0Ref
Molar Mass, H2	MH2
Molar Mass, O2	MO2
Area of Electrode	Ael
Nominal Current	iNom
Nominal Voltage	UNom

Name: in1
Comment: Signal Input
Dimension: Scalar

Declaration Condition	
Protected	☐
Variability	Variable
Display as Parameter	☐
Display as Result	☑

Figure 10 - Connectors and Components tabs

On the “Behavior” tab a list of equations and algorithms can be set to describe the behavior of the model. It is on this tab that every equation set in this section goes. All variables must be input in the same notation as the properties were defined before, so the number of equations and variables match by the time the simulation is to run. Some parameters/variables that are input, also have to be related to the block’s notation, e.g. pO_2 = $portO_2.p$. In this example, pO_2 which refers to the oxygen pressure in the anode inlet, is going to be a result on the simulation, so for it to work, it must be related to the model’s notation, so it recognizes it and gives feedback upon request. On the other hand, $portO_2.p$ is the pneumatic port set before for the oxygen inlet at the anode, “.p” is actually the way to refer to a certain variable/parameter inside a component (model, connector, etc.). Still on this behavioral parameterization, the algorithms can be used, for example, to check for common mistakes, like the usage of the correct fluids in each connection. In the event of incorrect fluid usage, an algorithm like this can trigger a message to show up in the output screen. Next is “Modelica Code” tab. This is the heart of the model. Everything that can be done in all the other tabs, shows up here. From the declaration of all the variables and parameters used, to all the models and their behavior. This can serve as the interface for quicky editing some line of code, or to hardcode every aspect of the model.



```
pO2 = portO2.p;
pH2 = portH2.p;
pH2O = pAtm + portH2O.p;

//Control System

der(U) = 1/Tc*(PSet-Pin)/PelNom;

//Electrochemical Model
U = Uocv + Uohmic + Uact;

    Uocv = (Urev + Rn*T/(2*Fc)*ln(pH2/1'bar'*(pH2O/1'bar')^0.5))*ta
        Urev = 1.5184-1.5421e-3*T+9.523e-5*T*ln(T)+9.84e-8*T^2;

    Uohmic = if noEvent(j>0) then Rr*Ael*j else 0;
        Rr = RrNom*exp(-kT*(1/TNom-1/T));

    der(Uact) = 1/Td*(Rn*T/(0.5*2*Fc)*ln((if noEvent(j/j0>1) then j
        j0 = j0Ref*exp(EAct/Rn*(1/TNom-1/T));
```

```
model Electrolyzer "Electrolyzer"
    input SignalBlocks.InputPin in1 "Signal Input" annotation(...);
    Hydraulics.PortCompound portH2O "Hydraulic Port" annotation(...);
    Pneumatics.PortCompound portH2 "Pneumatic Port" annotation(...);
    Pneumatics.PortCompound portO2 "Pneumatic Port" annotation(...);
    Pneumatics.Connection connO2(
        redeclare replaceable function Fluid = Pneumatics.Fluids.Gases.Oxygen,
        p0=pA0,
        T0(fixed=false)=TA0);
    Pneumatics.Connection connH2(
        redeclare replaceable function Fluid = Pneumatics.Fluids.Gases.Hydrogen,
        p0(fixed=true)=pC0,
        T0(fixed=false)=TC0);
    Hydraulics.Connection connH2O(
        redeclare replaceable function Fluid = Hydraulics.Fluids.Miscellaneous.H2O,
        p0(fixed=false),
```

Figure 11 - Behavior and Modelica Code Tabs

Furthermore, there are two more tabs, “Documentation” and “Security”, where one can write a document (to describe the model and its functionalities, or even reference the literature used, for example) and define the security settings and accessibility to the “TypeDesigner”, respectively.

After various iterations, a final model was designed (Figures 12 and 13).

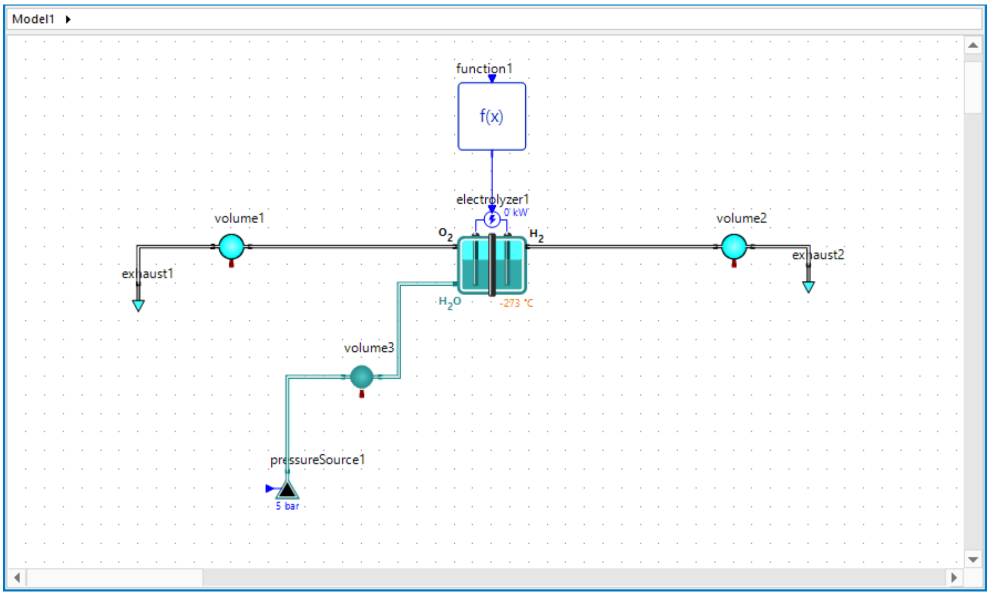


Figure 12 - Final Electrolyser Model (connected to standard elements, to test and measure results)

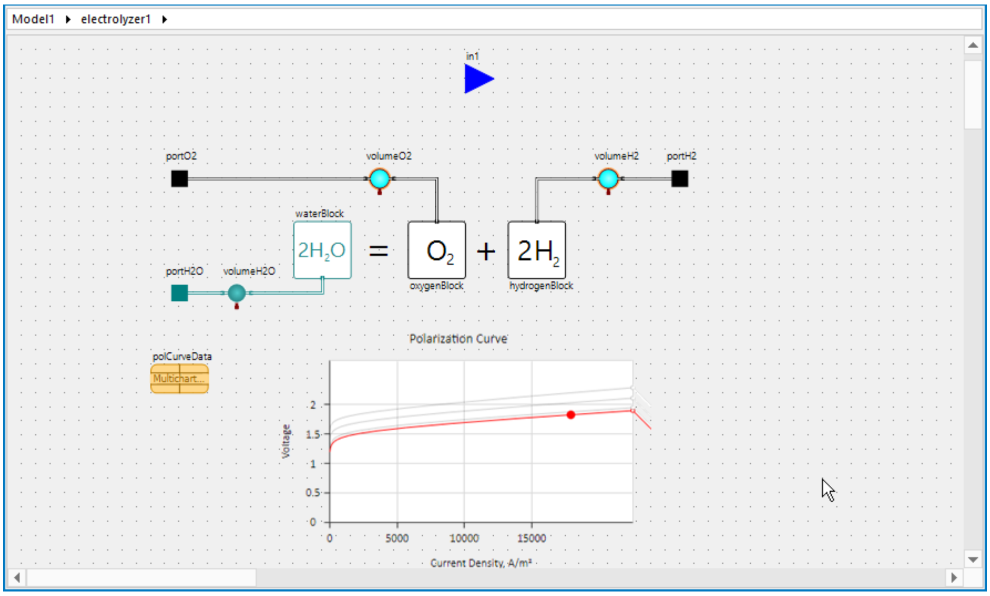


Figure 13 - Final Electrolyser Model: Inside the compound overview

Figure 12 presents a simple assembly of the electrolyser model connected to basic elements. It was used like this just to make tests and measure results, to benchmark the modeled electrolyser with some commercial applications. From Figure 12, the compound breakdown is represented. The properties of the blocks provide the variables/parameters for the equations: water, oxygen and hydrogen blocks, connectors and ports are very self-explanatory, but “in1” is the electrolyser power inlet. Inside the compound is also a representation of the polarization curve. In Figure 13, the red dot represents the point of operation on the polarization curve for the last simulation that was ran. The results will be provided throughout Chapter 4.

3.2 Factory Assembly

The electrolyser is not the only equipment which had to be modeled, to optimize the factory and its green hydrogen production. There are other parts of the plant that the built-in models do not account for. The water treatment section (ion exchange membranes) as well as the VPSA unit are some good examples of that. Nonetheless, for simplification purposes, in the ion exchange membranes the project considers no mass transfer losses, so the water flow is the same in the inlet and outlet of that unit. For the VPSA, the project considers a factory of recovery of 95%, which is a little bit more conservative than the literature’s 98%.

3.2.1 Power Input

As it will be further explored in Chapter 4, electricity costs can vary throughout time and to optimize the cost of production, it is important to buy the lowest priced electricity. This happens when there is high availability and low demand. More detailed information and a deeper analysis on this will be provided in the next section.

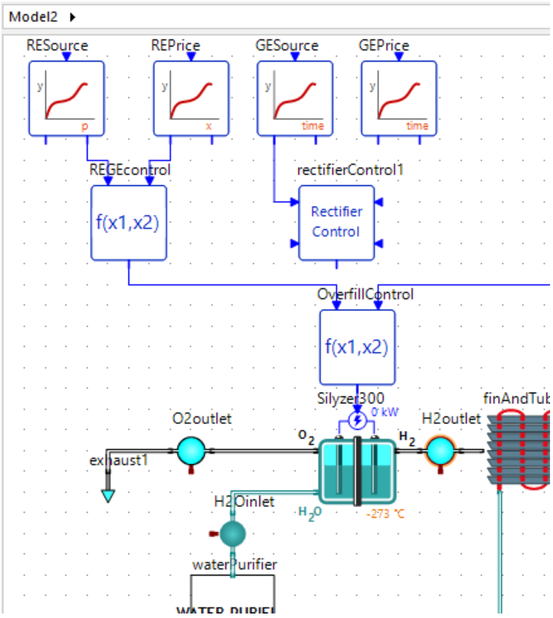


Figure 14 - Power Input

For the factory model there are two main things to consider. The electricity price and the fraction of storage available. These are the conditions that control production. For that reason, a control system was designed as shown in Figure 14. “RESource”, “REPrice”, “GESource” and “GEPrice” stand for electricity from renewable sources (availability), price of renewable electricity, electricity from the grid and grid electricity price, respectively. The block “REGEControl” contains an IF function and controls if whether the energy to feed the electrolyser comes from renewable sources or the grid. It decides based on the renewable electricity and price. The “OverfillControl” block is a controller that acts upon the pressure of the stored hydrogen. If, for any reason, the tank is about to be full, it stops production. It is important to point that the electrolyser runs on DC Power, which is compatible with electricity from renewable sources. In the case of using grid power, there is the need of using a rectifier to get the current from AC to DC.

3.2.2 Water Input

As stated in Section 2, the water required for this process is 9kg per 1kg of H_2, but that is not the only requirement. The water conductivity must stay between 0.1 – 10 $\mu S \cdot cm^{-1}$ so it does not interfere with the PEM conductivity.

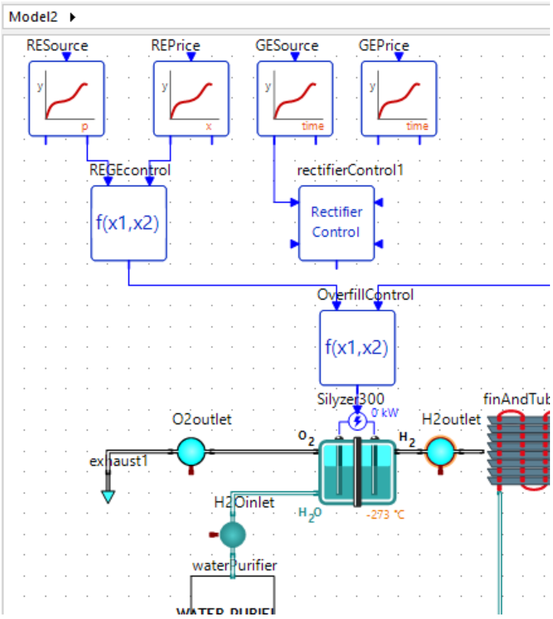


Figure 15 - Water Feed

From Figure 15, it is possible to observe that water comes from a water source (can be a tank or even a local water supplier) at atmospheric conditions. The centrifugal pump will feed the water to the water purification unit at 5 bar. As stated before, there will not be considered any mass transfer loss, so the mass flow on both ports of the “WaterPurifier” block are the same (portin.mdoth2o=portout.mdoth2o; “mdot” stands for mass flow). After the stream of water being properly degassed and deionized, it enters the electrolyser pressurized at 5 bar which is also the pressure of operation for the anode side.

3.2.3 Hydrogen Purification, Compression and Storage

The VPSA unit is not mandatory. As stated before, the hydrogen purity requirements are not transversal, but rather depend on the specific application. For mobile applications, such as FCV’s, a very high pure content of hydrogen is required (ISO 14687:2019), but for other applications, there is no need for that kind of purity. Something that must be accounted as well is the type of electrolysis and the purity of the outstream hydrogen. Some manufacturers guarantee ultra-pure hydrogen 5.0 which corresponds to a purity of 99.999% [7]. Nevertheless, it is necessary to dry the hydrogen stream before compressing it. For that reason, a heat exchanger is added right after the electrolyser hydrogen outlet (Figure 16).

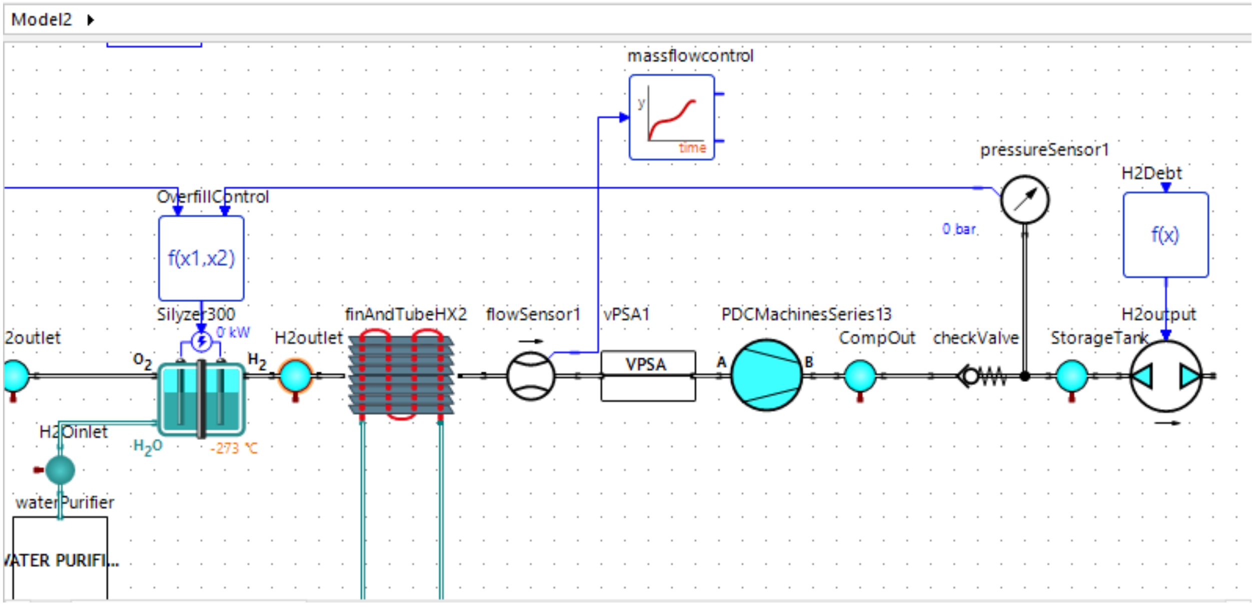


Figure 16 - Hydrogen purification, compression and storage

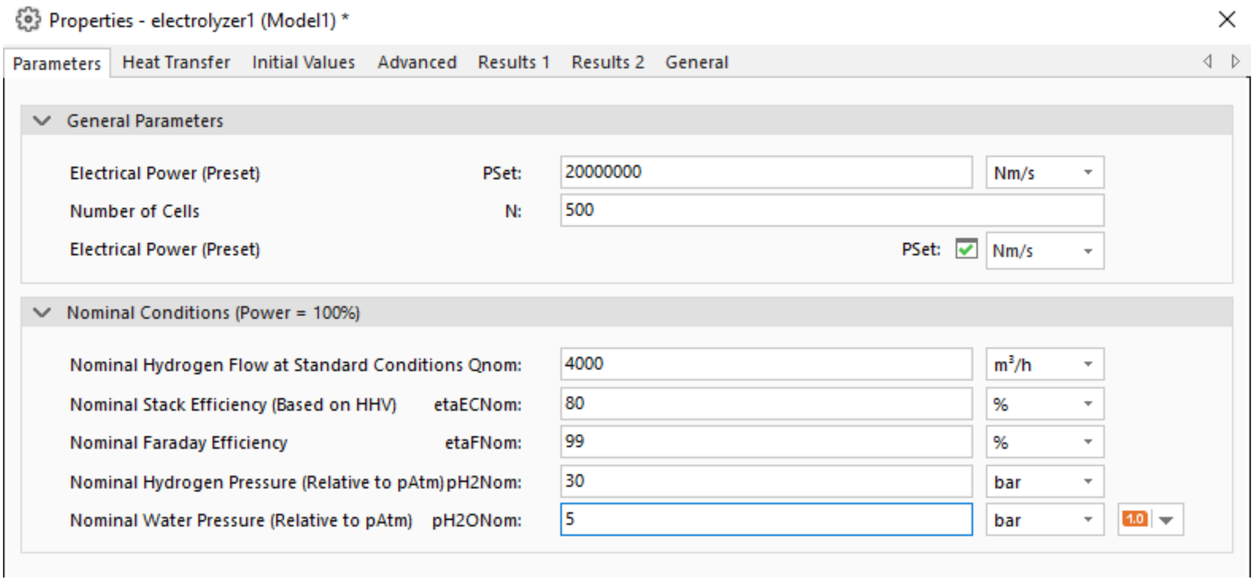
As the products form in water, the hydrogen stream is saturated with water. The heat exchanger will remove most of the water, but to further dry the hydrogen stream, the VPSA unit must be used. The flow sensor connecting the heat exchanger to the VPSA gives information about the mass flow. That way the fraction of water removed in the first drying step can be calculated, as well as the remaining hydrogen purity. If there is the need of getting the water below 500 ppm, then the stream shall go on the VPSA, otherwise, it can skip it and go directly to the compression stage. The VPSA was not fully modeled. The only real parameterization it has is that its recovery is of 95 %. That means that on the behavior, it was set that portout.h2=0.95·portin.h2. In the next step, the best fit for the compressor stage is the PDC Series 13. It is a diaphragm compressor that can get the desired discharge pressure, 250 – 300 bar, without a cycle of compressors [43]. PDC is an American company, number one supplier of hydrogen compressors in the market with over 350 compressor units sold worldwide (PDC Machines' website). This type of compressor has a built-in 3 stage cycle, which allows for very high discharge pressures (up to 1000 bar), without the risk of contamination and temperature control with built in heat-exchangers. As for the last part, the storage is assured by stainless-steel vessels The sizing is presented in the results.

4 Results and discussion

In this section, the results for the electrolyser tests are presented and from then, the sizing of the factory and equipment. After that, a technical analysis shall be presented, ending with a project of investment analysis, with the calculation of the various NPV for the different operation scenarios.

4.1 Electrolyser Results

Technical specifications of selected electrolysers from well-known manufacturers were introduced into the simulator; the comparison of these technical specifications with the results from the simulator was also performed. The selected electrolysers were 17.5 MW Silyzer 300 from Siemens (PEM electrolyser) and 20 MW module from Thyssenkrupp (alkaline electrolyser). Double-clicking the electrolyser, opens its properties, where one can find the parameterization window (Figure 17).



General Parameters

Electrical Power (Preset) PSet: 20000000 Nm/s
Number of Cells N: 500
Electrical Power (Preset) PSet: ☑ Nm/s

Nominal Conditions (Power = 100%)

Nominal Hydrogen Flow at Standard Conditions Qnom: 4000 m³/h
Nominal Stack Efficiency (Based on HHV) etaECNom: 80 %
Nominal Faraday Efficiency etaFNom: 99 %
Nominal Hydrogen Pressure (Relative to pAtm) pH2Nom: 30 bar
Nominal Water Pressure (Relative to pAtm) pH2ONom: 5 bar

Figure 17 - Parameters window for electrolyser simulation

After filling every parameter with typical values from other electrolyser datasheets, like the 20 MW power input, 500 cells which account for a very high value of current density, the expected hydrogen flow at standard conditions of 4000 $m^3 \cdot h^{-1}$ with a stack efficiency of 80 %. As for the results, the temperature of operation was 80 °C, the hydrogen output pressure of 30 bar, and as for the polarization curve, it can also be obtained as well as the operating values for the voltage and current density (Figure 18). The mass flow stayed constant at 0.113 $kg \cdot s^{-1}$, once the power input remained constant as well (Appendix A).

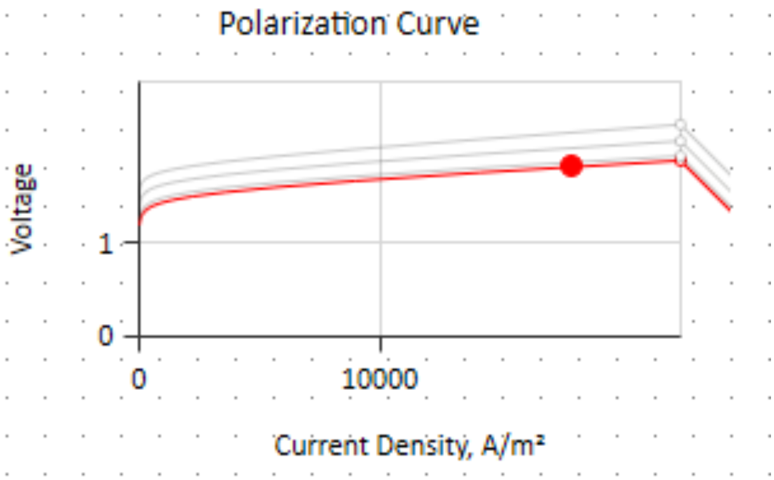


Figure 18 - Polarization Curve

The values for the cell voltage and current density are 1.82 V and 2.19 A·cm^{-2}, respectively. The mass flow value can naturally be converted into kg·h^{-1} by simple multiplying it by 3600 s. Hence, a value of 406.8 kg·h^{-1} is reached and from this, it is possible to size the factory and further progress into more detailed analysis.

4.2 Sizing

Starting from the water perspective, the water consumption of this plant would be of 3661.2 kg·h^{-1}, just to feed the electrolyser, not accounting for the water to be used in the heat exchanger. The power supply would be of 20 MW, either directly provided by a renewable source, or through the grid with a rectifier. As for the compressor, PDC Machines advertises to have this type of compressors already installed, with both these mass flows and discharge pressures. The last thing would be the storage. Using stainless-steel vessels would be the most interesting option at this point. In the extreme scenario of working a 100 % load and having to store 3 full days of production, the result would be roughly 1500 m^3, assuming a density of 20 kg·m^{-3} for the hydrogen at 300 bar. According to [60], the storage solution could be 1 big vessel with 13.7 m diameter and 11 meters height, providing 1625 m^3, or two smaller vessels, each with 819 m^3 (10.7 m diameter and 9.1 m height). The design temperature should be at least 10 °C above the operation temperature. The design pressure should be 10 % above the maximum operating pressure (about 330 bar). The vessels must include floating or expansion roofs and considering such a great capacity, it should be built as vertical tanks on concrete foundations. Finally, these tanks should not be filled above 90 %.

4.3 Financial Analysis

For the financial analysis, the difference between alkaline and PEM electrolysis will be further explored, this time comparing the financial implications of each technology. As the electricity costs represent more than half of the total overall costs, the best way to start this analysis is to analye the electricity market.

4.3.1 MIBEL

MIBEL is acronym for Iberian electricity market. With the establishment of this market, a market operator has been formed as well – OMI (Iberian Market Operator). This operator has two sections OMIE which is the Spanish center, responsible for intraday market management and OMIP, the Portuguese center responsible for forward markets [61]. OMIP provides with a lot of data either from the past or even for the price of next year's electricity contracts. With this free data provided online on OMIP website, some charts were created to try and preview how electricity costs fluctuate throughout the year. Monthly average electricity costs were calculated considering everyday electricity costs since 2018, as well as the values for the highest and lowest prices registered in that month, and the results were displayed yearly in three charts as follows (Figures 20, 21 and 22).

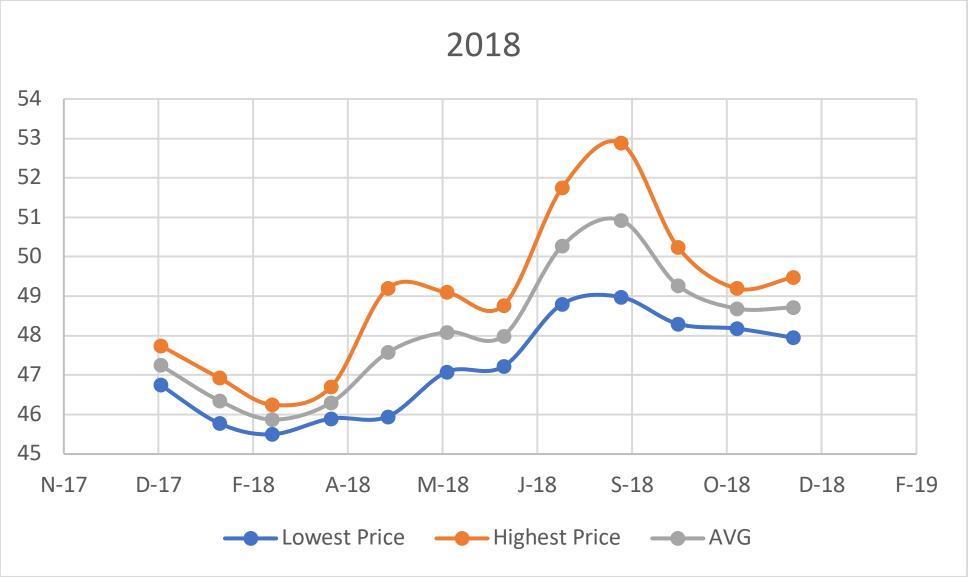


Figure 19 - 2018 historic electricity prices (lines were added just for guiding the eyes)

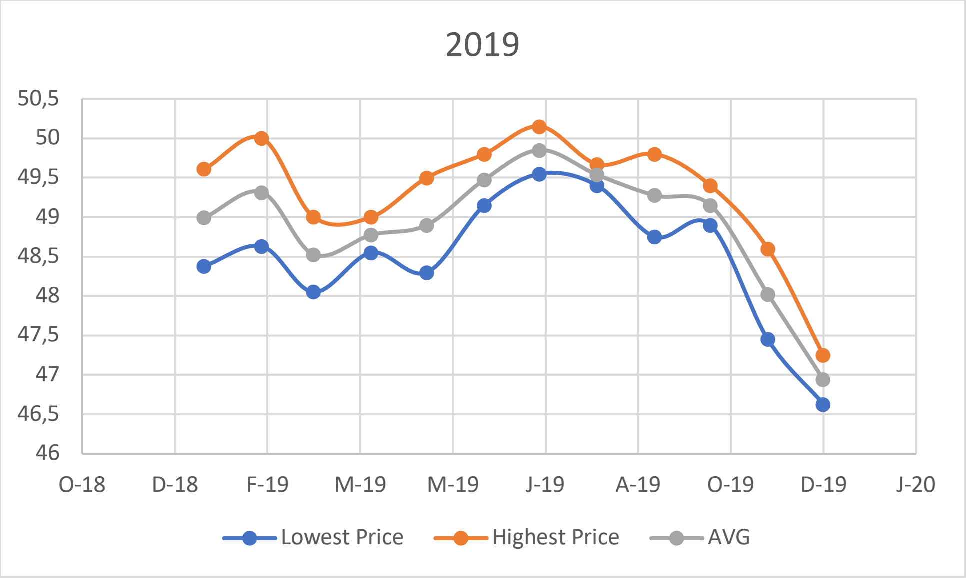


Figure 20 - 2019 historic electricity prices (lines were added just for guiding the eyes)

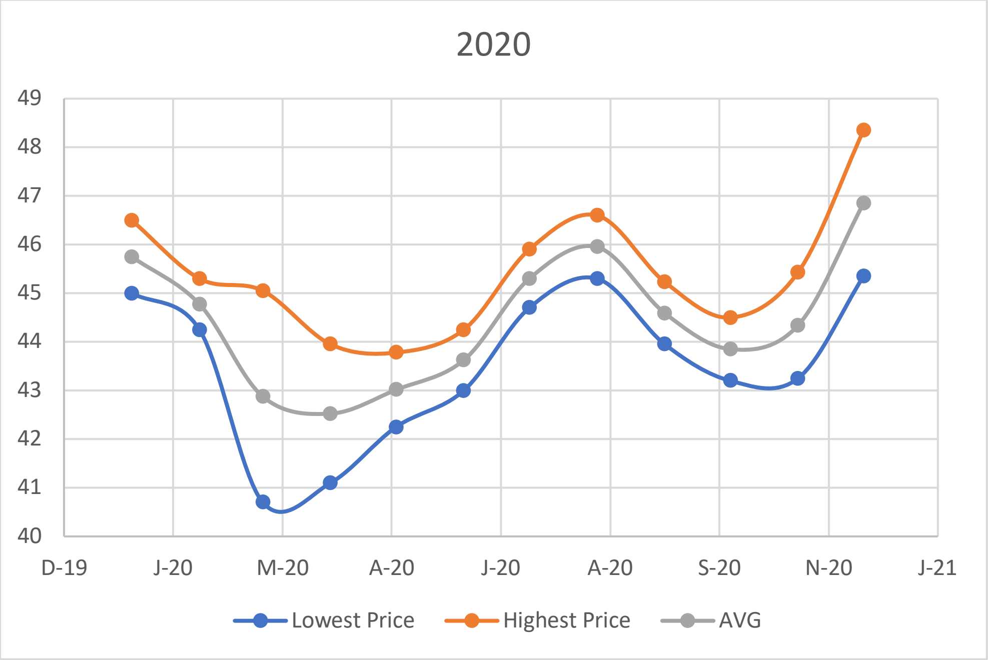


Figure 21 - 2020 historic electricity prices (lines were added just for guiding the eyes)

The main objective with this preliminary analysis on the historic electricity average prices is to try to determine any pattern that might occur during the year. It might not be straightforward, but there is a small pattern in electricity price throughout the year. There are some months when the availability is higher than the demand. In those cases, the electricity is going to be cheaper. There are other months when there is great demand, so the electricity price goes up. Figure 23 helps demonstrate this rationale.

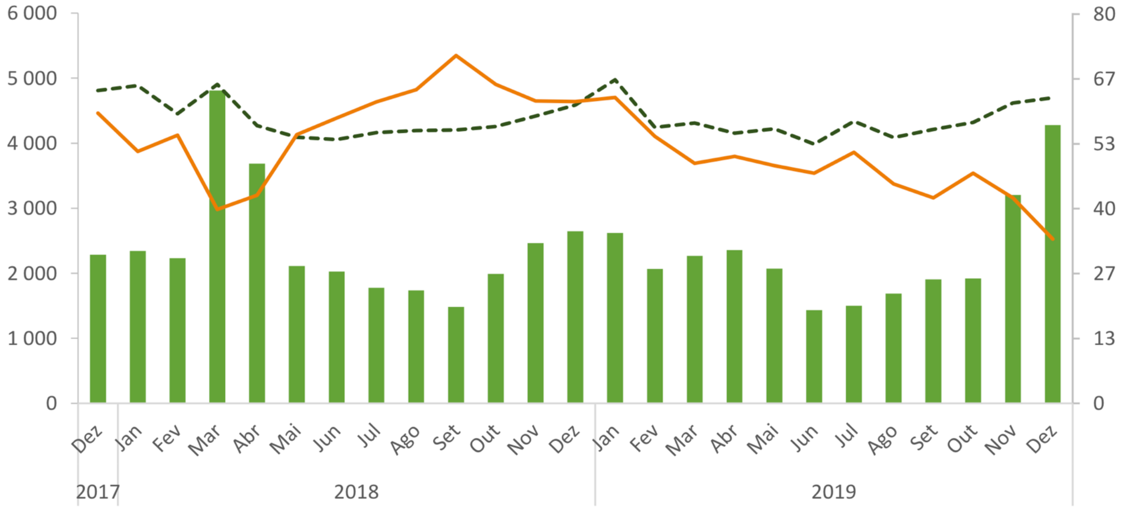


Figure 22 - left y-axis - Electric Energy (GWh); right y-axis - Price (€/MWh); light green bars - Renewable energy generation (GWh); orange line - Market price (€/MWh); dark green line - Consumption (GWh) – (extracted from [62])

In this case it is apparent that the market price is higher when the renewable energy generation is low, which is during summertime (from May to September) in both 2018 and 2019. On the other hand, market price is lower in wintertime, where the renewable energy peaked in March and April 2018 and again in November and December 2019. In both these cases the electricity price was around 40 €·MW^{-1}h^{-1} which is low compared to the usual market price. Analysing the three graphs from Figures 20 to 22 in more detail, it can be concluded that, on average, half of the year the electricity is below the year's average price and the other half is above. Also, the average difference between the highest and lowest prices within a given month, (considering the data provided from OMIP comprehended between 1/2018 and 03/2021) is 1.8866 €·MW^{-1}h-1. Since the load electrolysers assumed for the electrolysers is 40 % - 100 %, the hydrogen plant will buy hydrogen whenever it is cheap.

4.3.2 CAPEX

CAPEX, or Capital Expenditures, is the amount of financing needed to acquire every equipment and infrastructure needed for the process to take place. In this case, all equipment like the electrolysers, compressors, rectifiers and storage tanks will account for that price, but the infrastructural part will be neglected. Table 5 gives information on all CAPEX values. The values for the PEM electrolyser, rectifier and compressor were considered according to [63], the alkaline electrolyser capex is based on a conversation with an executive officer from Thyssenkrupp and finally, the storage tank is based on an estimate calculation from [64].

Table 5 - Table of CAPEX

PEM electrolyser ($/kW)	1 500
ALK electrolyser ($/kW)	500
Rectifier ($/kW)	130
Compressor ($/kW)	40
Storage Tank ($)	590 419

The value for the PEM electrolyser, rectifier and compressor CAPEX was extracted from [63], as for the alkaline electrolyser it was provided by one manufacturer. The storage tank CAPEX was calculated according to [64]. For the rest of this comparison, the two selected electrolysers are the 17.5 MW Silyzer 300 from Siemens (PEM) and the 20 MW module from Thyssenkrupp (Alkaline). The specifications for both equipment are shown in Table 6.

Table 6 - Specifications for both electrolysers

	Sylizer 300	**Thyssen 20 MW**
Nominal Power (MW)	17.5	20
# modules	24	-
efficiency (%)	75.5	82
max. H_2 output (kg/h)	396.375	492
H_2 purity (%)	99.9999	99.95
water consumption (L/kgH_2)	9	9
response time (min)	<1	>1
dynamics (%/s)	10	-
min. load (%)	>5	10

With these values, the only thing left to do in relation to CAPEX is to scale-up to the plant size, multiplying by the nominal power in each case (except for the storage tanks) and convert it to euros (Table 7).

Table 7 - Total CAPEX for both electrolyser + plants (in M €)

CAPEX	**Silyzer 300**	**Thyssen 20 MW**
Electrolyser ($)	26.25	10.00
Rectifier ($)	2.28	2.60
Compressor ($)	0.700	0.800
Storage Tank ($)	0.714	0.714
Total CAPEX ($)	29.23	14.11

Total CAPEX (€)	24 16	11.67
Total CAPEX + 20% mark-up (€)	28.99	14.00

These values will be used further on the calculation of the NPV, so a better understanding of the differences between technologies is deeper acknowledged. In the meantime, the main takeaway from the direct analysis is that the CAPEX for the PEM electrolysis is more than 2 times greater than the one for its alkaline counterpart, even though the nominal power is lower in the PEM technology (for this case).

4.3.3 OPEX

The Operational Expenditures typically include all fixed and variable costs associated to running the industrial facilities. This usually covers raw materials, equipment rentals, labour costs, etc. The OPEX considered for this project is presented on Table 8.

Table 8 - Table of OPEX

Fixed O&M ($/kW.y)	14.50
Fixed O&M ($/MW.y)	14 500
Variable O&M ($/MW.h)	0.51
Variable O&M ($/MW.y)	4 467
Cooling Water ($/m3)	0.02
Process Water ($/m3)	0.20

The electricity costs are not shown here due to their fluctuation throughout the year. Using a single price for the electricity for the entire year would not correspond to a very accurate analysis. Fixed and Variable Operation & Maintenance values were extracted from [63] and for both cooling and process water from [64]. With these values, the OPEX was calculated on a yearly basis, for operation at different loads (40 – 100 %). An example of that type of calculations is represented on Table 9.

Table 9 - OPEX, operation time, production and durability calculation

Load	0,4
Fixed O&M ($/y)	116 000
Variable O&M ($/y)	35 740
Total O&M ($/y)	151 740
Total O&M (€/y)	125 428
Total Operation (h/y)	3 504
Total Production (kg/y)	1 723 968
Durability (y)	17

These tables were calculated for each load, from 40 – 100% for both electrolysers' technologies. All tables can be consulted in the appendix.

4.3.4 Revenues and Expected Cash-Flows

To calculate the expected revenues some key assumptions had to be made. These assumptions are represented in table 10 along with the sources of information. As a disclaimer, the hydrogen price set on this assumption table is neither the lowest market price nor the typical selling price of green hydrogen. It is a valuable not so low that it would make the process completely unviable, but not so high that the market won't absorb it.

Table 10 - Key Assumptions (with references)

1 USD (EUR)	0.8266	[65]
H_2 Price 2021 (€/kg)	2.7	[2]
H_2 Price Decrease (%/y)	0.04	[2]
Electricity Price (€/MW.h)	67.88	[66]
Electricity Price Decrease %/y	0.0298	[66]
Discount Rate (%)	10%	

The discount rate is only to be used for the NPV calculation. With this and having the total annual production (in kg), the gross income can be calculated. Also, with the MIBEL analysis from the first point of this section, a good estimate for the electricity prices throughout the year can be considered. The cells presented in Table 11 are calculated as follows.

$$H_2\ Price\ (€ \cdot \mathrm{kg}^{-1}) = X - (X \cdot y \cdot z) \tag{22}$$

where X is H_2 Price 2021 (€/kg) and z the H_2 Price Decrease (%/y), from the key assumptions and y is the year period, starting in 1 and ending in the last year of durability for each load of operation.

$$Revenues\ (€ \cdot \mathrm{y}^{-1}) = Total\ Production\ (\mathrm{kg} \cdot \mathrm{y}^{-1}) \cdot Hydrogen\ Price\ (€ \cdot \mathrm{kg}^{-1}) \tag{23}$$

$$Electricity\ Price\ (€ \cdot \mathrm{MW}^{-1}\mathrm{h}^{-1}) = Ep \pm Hg - (Ep - Hg) \cdot y \cdot Epd \tag{24}$$

where Ep is the electricity price from the key assumptions table, Hg is half the average gap (difference between highest and lowest monthly electricity prices) from section 4.3.1 and Epd is the electricity price decrease from the key assumptions table. The fact that

Hg can be some or subtracted has to do with the load. Below 50% load it is subtracted, above that it is added to the electricity price.

$$Electricity\ Costs\ (€ \cdot y^{-1}) = Epl \cdot P \cdot Op \cdot \%Tl + Eph \cdot P \cdot Op \cdot \%Th \tag{25}$$

where Epl is the "low-cost electricity" ($€ \cdot MW^{-1}h^{-1}$) corresponding to the value when the electricity price (Eq. (24)) is calculated by subtracting Hg), P is the nominal power (MW), Op is the total operation time ($h \cdot y^{-1}$), $\%Tl$ is the percentage of time working at Epl. On the other hand, Eph and $\%Th$ are the "high-cost electricity" and percentage of time working in this regime, sharing the same units as their lowest values counterparts. Naturally, $\%Tl$ + $\%Th$ = 1.

$$\text{Cashflow}\ (€ \cdot \text{y}^{-1}) = \text{Revenues}\ (€ \cdot \text{y}^{-1}) - \text{OPEX}\ (€ \cdot \text{y}^{-1}) - \text{Electricity Costs}\ (€ \cdot \text{y}^{-1}) \tag{25}$$

The full tables can be consulted in the appendix. With these results, it is finally possible to calculate the NPV for both technologies.

4.3.5 Project Net Present Value

Considering the CAPEX, the cashflows and the discount rate from the key assumptions table, it is possible to calculate the project's NPV for both PEM and alkaline electrolysis. NPV is used to calculate the current total value of a future stream of payments discounted to the present. NPV equation is as follows:

$$\text{NPV}\ (€) = -\text{CAPEX} + \sum_{\text{t}=1}^{\text{n}} \frac{\text{CF}}{(1+\text{i})^{\text{t}}} \tag{26}$$

where CF is the cash flow for period t (yearly). Table 11 exhibits the results for both electrolysers operating at the different loads.

Table 11 - NPV results (in M€)

LOAD	Thyssen 20MW	Silyzer 300
0.4	(15.28)	(27.55)
0.5	(15.96)	(27.93)
0.6	(16 34)	(28.17)
0.7	(16.73)	(28.36)
0.8	(16.97)	(28.46)
0.9	(17.07)	(28.47)
1	(17.02)	(29.03)

From the direct analysis of Table 11, one can quickly realise this does not look like a good investment, once all results are negative. Nonetheless, some observations can be appointed to these results. Sylizer is still overall more expensive than Thyssenkrupp's alkaline model, although that would be expected, as stated in section 2.2. This values of NPV are accounted for the chosen value for selling the hydrogen. Another analysis was made, using an iteration for the price of hydrogen to find the actual selling price that would start to yield profit for the process operation. The results are shown in Table 12.

Table 12 - NPV results for the cost-based analysis (in M€)

LOAD	**Thyssen 20MW**	**Silyzer 300**
0.4	(4.06)	(7.41)
0.5	(2.05)	(3.47)
0.6	(0.518)	(0.700)
0.7	1.04	2.47
0.8	2.39	5.14
0.9	3.46	7.18
1	3.45	7.75

The iteration that consisted in these results for the NPV were Hydrogen Selling Prices of 4 €$\cdot$kg^{-1} and 5.5 €$\cdot$kg^{-1} for Thyssenkrupp's 20MW module and Silyzer 300, respectively. This hydrogen prices are considered for year 0, after year 1 the "hydrogen price decrease" rate from the key assumptions table is used, according to Eq. (22).

5 Conclusions

This dissertation concerned the development of a simplified phenomenological model of an electrolyser using the simulation platform SimulationX from ESI-Group. The results were in line with the literature for the mass flows as well as for the operating voltage and current density. It was then to integrate this electrolyser within a hydrogen factory. Concerning the best performing electrolyser – Thyssenkrupp's 20 MW – it was computed a hydrogen production mass flow of 406.8 kg·h^{-1} and operating voltage and current density of 1.82 V and 2.19 A·cm^{-2}.

On the economical side, analyzing the data for the last 3 years of the Iberian Electricity Market prices, it was drawn an average trend for the electricity price, for each year; it was possible to identify that, on average, one year has 6 months with cheaper electricity and the other half of the year with more expensive electricity. Two different electrolysers were considered to compare the operation economical balance between a PEM and an Alkaline electrolysis. The selected equipment was the Silyzer 300 (PEM) and Thyssenkrupp's 20 MW module (Alkaline). The CAPEX and OPEX was determined for each technology where Silyzer is far more expensive per power unit than Thyssenkrupp's 20 MW. Assuming different market hydrogen prices, it was possible to calculate revenue streams and, thus, the net present value for the overall project. Firstly, considering a selling price of 2.7 €·kg^{-1} negative NPV in the range of 17 M€ – 30 M € were calculated, but for selling prices of 4 €·kg^{-1} and 5.5 €·kg^{-1} for alkaline and PEM production, respectively, the NPV started to be positive, yielding profits. In order to be financially feasible to sell the hydrogen at 2.7 €·kg^{-1}, it would be necessary to receive public funding. This seems adequate, once otherwise the market would not absorb the produced hydrogen at higher prices and the Portuguese government is allocating more than 700 M€ to finance this kind of initiatives.

6 Assessment of the work done

6.1 Objectives Achieved

The main objective set for this dissertation was to assert the viability of the project. This objective is divided into two parts. The technical feasibility and financial sustainability. As for the first part, the objective was partly accomplished, once the electrolyser model was built, but to determine the technical feasibility more hardcoded components had to be created and more simulations had to be run. In the financial analysis, there are some aspects that can be optimized. A more robust method of predicting the electricity price could be created. As the electricity costs account for 80% of the overall expenses, it is important to develop a model that can predict the next energy prices. This would allow for a smart buy, reducing the overall costs and optimizing the system's net-profit. This could be done using machine learning, continuously reading and analyzing data from OMIP and also taking into consideration the electricity availability and demand.

6.2 Final Assessment

The hydrogen has been increasingly gaining exposure and popularity through the media, governmental policies and a lot of R&D. It seems like todays 70 Mton market is to grow exponentially in the next few years. This makes it very thrilling to be working where the center of attentions is, but, at the same time, the lack of available information made it difficult for me to progress with rhythm. I started this dissertation with a lot of enthusiasm and motivation, but sometimes it would be hard to stay this way, once I was facing a lot of difficulties. Also, the fact that this is so recent, it also means that there is practically nothing done. From production upstream with the water input requirements, methods to treat it, the power input and the use of rectifiers. Also downstream, the challenge of purifying the hydrogen stream with heat exchangers and PSA units, to the compression stage maintaining acceptable temperatures to its storage and distribution. Sometimes this can be positive once working on a blank canvas enhances creativity, but it also generates a lot of confusion for the problem's great level of complexity.

Finally, the necessity of hardcoding in modelica was something that came a little unexpected and I did not have the time to properly learn this hard skill in order to fully demonstrate my potential and capacities.

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8 Appendix A - mass flow results from simulation

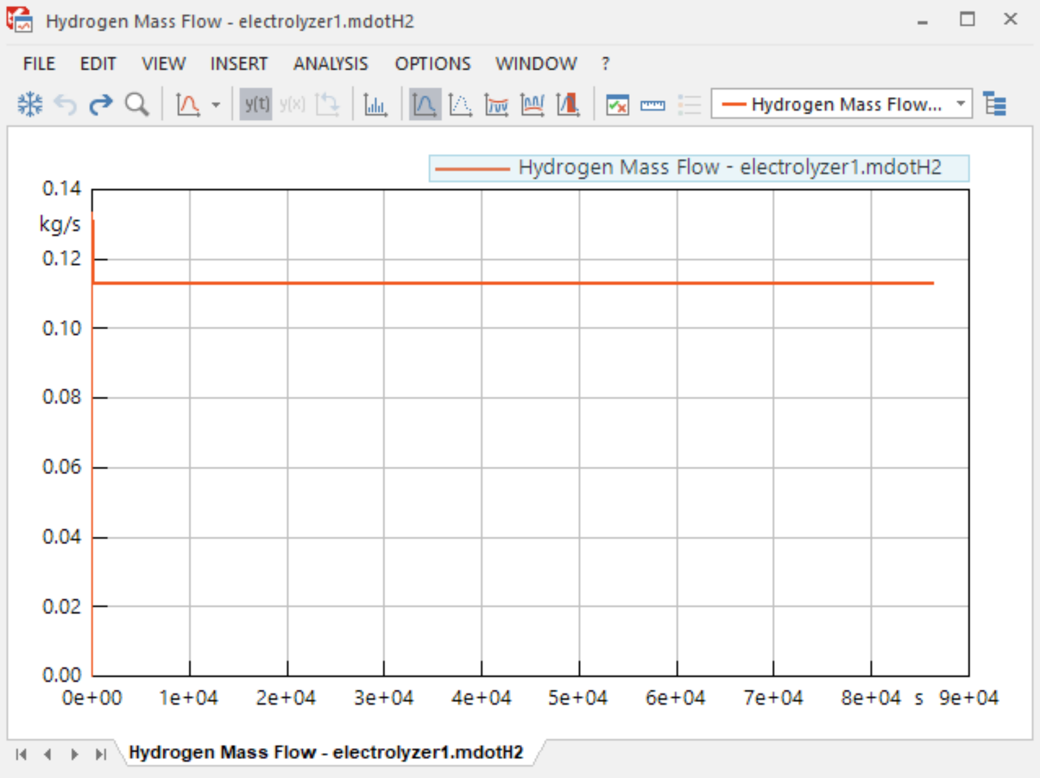


Figure 23 - Mass flow results for the 20 MW electrolyser simulation

9 Appendix B - OPEX for Silyzer 300 different loads

Table 13 - Opex for Silizer 300 at different loads

Silyzer 300			
Load			0,4
Fixed O&M ($/y)	$	101 500,00	
Variable O&M ($/y)	$	31 273,20	
Total O&M ($/y)	$	132 773,20	
Total O&M (€/y)		109 750,33 €	
Total Operation (h/y)		3 504	
Total Production (kg)		1 388 898	
Durability (y)		17	
Load			0,5
Fixed O&M ($/y)	$	126 875,00	
Variable O&M ($/y)	$	39 091,50	
Total O&M ($/y)	$	165 966,50	
Total O&M (€/y)		137 187,91 €	
Total Operation (h/y)		4 380	
Total Production (kg)		1 736 123	
Durability (y)		14	
Load		0,60	
Fixed O&M ($/y)	$	152 250,00	
Variable O&M ($/y)	$	46 909,80	
Total O&M ($/y)	$	199 159,80	
Total O&M (€/y)		164 625,49 €	
Total Operation (h/y)		5 256	
Total Production (kg)		2 083 347	
Durability (y)		11	
Load		0,70	
Fixed O&M ($/y)	$	177 625,00	
Variable O&M ($/y)	$	54 728,10	
Total O&M ($/y)	$	232 353,10	
Total O&M (€/y)		192 063,07 €	
Total Operation (h/y)		6 132	
Total Production (kg)		2 430 572	

Durability (y)		10	
Load		0,80	
Fixed O&M ($/y)	$	203 000,00	
Variable O&M ($/y)	$	62 546,40	
Total O&M ($/y)	$	265 546,40	
Total O&M (€/y)		219 500,65 €	
Total Operation (h/y)		7 008	
Total Production (kg)		2 777 796	
Durability (y)		9	
Load			0,9
Fixed O&M ($/y)	$	228 375,00	
Variable O&M ($/y)	$	70 364,70	
Total O&M ($/y)	$	298 739,70	
Total O&M (€/y)		246 938,24 €	
Total Operation (h/y)		7 884	
Total Production (kg)		3 125 021	
Durability (y)		8	
Load			1
Fixed O&M ($/y)	$	253 750,00	
Variable O&M ($/y)	$	78 183,00	
Total O&M ($/y)	$	331 933,00	
Total O&M (€/y)		274 375,82 €	
Total Operation (h/y)		8 760	
Total Production (kg)		3 472 245	
Durability (y)		7	

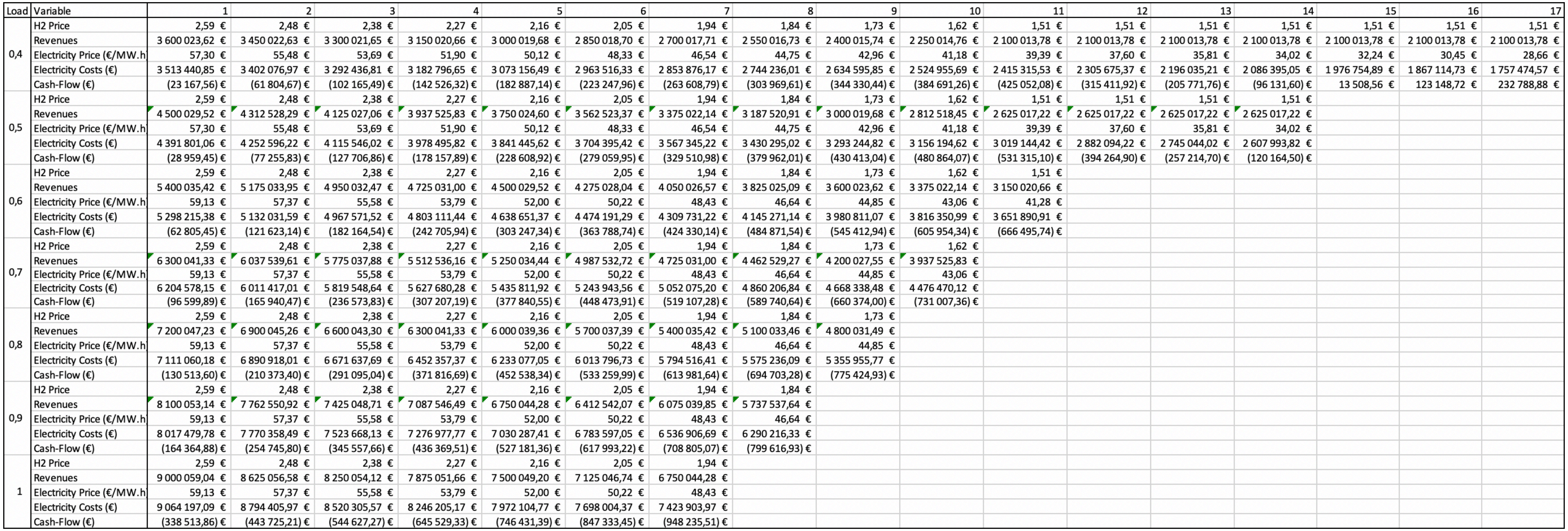
10 Appendix C – OPEX for Thyssenkrupp’s 20 MW module at different loads

Table 14 - Opex for Thyssenkrupp's 20 MW model at different loads

Thyssenkrupp's 20MW			
Load			0,4
Fixed O&M ($/y)	$	116 000,00	
Variable O&M ($/y)	$	35 740,80	
Total O&M ($/y)	$	151 740,80	
Total O&M (€/y)		125 428,95 €	
Total Operation (h/y)		3 504	
Total Production (kg)		1 723 968	
Durability (y)		17	
Load			0,5
Fixed O&M ($/y)	$	145 000,00	
Variable O&M ($/y)	$	44 676,00	
Total O&M ($/y)	$	189 676,00	
Total O&M (€/y)		156 786,18 €	
Total Operation (h/y)		4 380	
Total Production (kg)		2 154 960	
Durability (y)		14	
Load		0,60	
Fixed O&M ($/y)	$	174 000,00	
Variable O&M ($/y)	$	53 611,20	
Total O&M ($/y)	$	227 611,20	
Total O&M (€/y)		188 143,42 €	
Total Operation (h/y)		5 256	
Total Production (kg)		2 585 952	
Durability (y)		11	
Load		0,70	
Fixed O&M ($/y)	$	203 000,00	
Variable O&M ($/y)	$	62 546,40	
Total O&M ($/y)	$	265 546,40	
Total O&M (€/y)		219 500,65 €	
Total Operation (h/y)		6 132	

Total Production (kg)		3 016 944	
Durability (y)		10	
Load		0,80	
Fixed O&M ($/y)	$	232 000,00	
Variable O&M ($/y)	$	71 481,60	
Total O&M ($/y)	$	303 481,60	
Total O&M (€/y)		250 857,89 €	
Total Operation (h/y)		7 008	
Total Production (kg)		3 447 936	
Durability (y)		9	
Load			0,9
Fixed O&M ($/y)	$	261 000,00	
Variable O&M ($/y)	$	80 416,80	
Total O&M ($/y)	$	341 416,80	
Total O&M (€/y)		282 215,13 €	
Total Operation (h/y)		7 884	
Total Production (kg)		3 878 928	
Durability (y)		8	
Load			1
Fixed O&M ($/y)	$	290 000,00	
Variable O&M ($/y)	$	89 352,00	
Total O&M ($/y)	$	379 352,00	
Total O&M (€/y)		313 572,36 €	
Total Operation (h/y)		8 760	
Total Production (kg)		4 309 920	
Durability (y)		7	

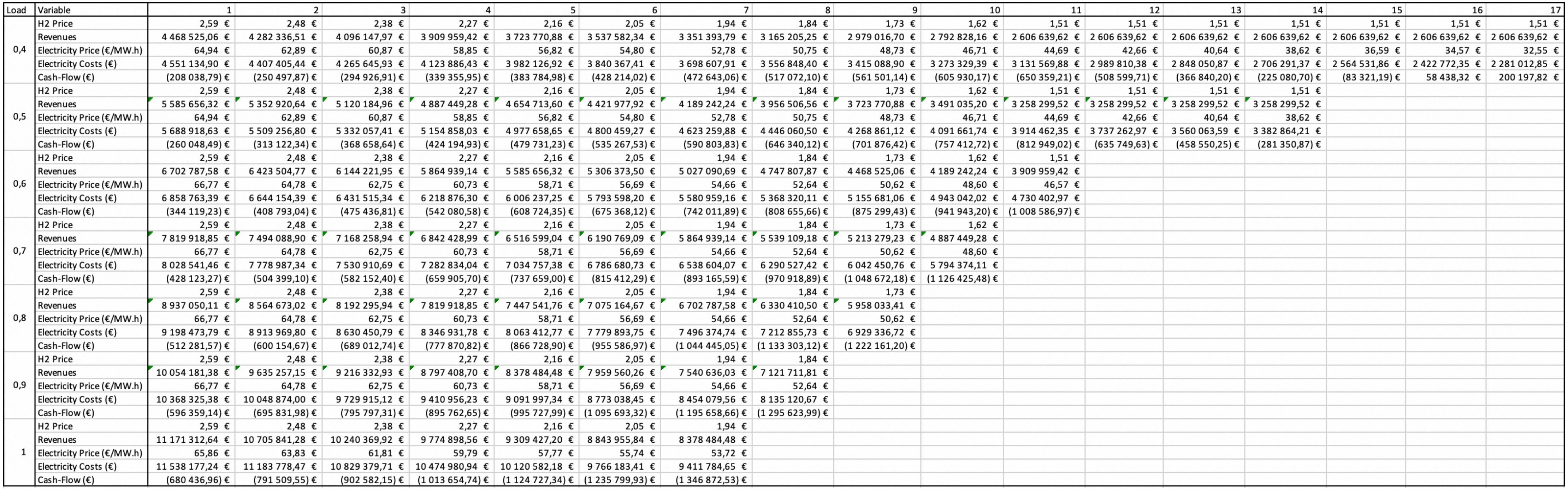
11 Appendix D - Silyzer 300 Cash-flows (2.7 €·kg^{-1})



Load	Variable	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0,4	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €	1,51 €	1,51 €	1,51 €	1,51 €	1,51 €	1,51 €	1,51 €
	Revenues	3 600 023,62 €	3 450 022,63 €	3 300 021,65 €	3 150 020,66 €	3 000 019,68 €	2 850 018,70 €	2 700 017,71 €	2 550 016,73 €	2 400 015,74 €	2 250 014,76 €	2 100 013,78 €	2 100 013,78 €	2 100 013,78 €	2 100 013,78 €	2 100 013,78 €	2 100 013,78 €	2 100 013,78 €
	Electricity Price (€/MW.h	57,30 €	55,48 €	53,69 €	51,90 €	50,12 €	48,33 €	46,54 €	44,75 €	42,96 €	41,18 €	39,39 €	37,60 €	35,81 €	34,02 €	32,24 €	30,45 €	28,66 €
	Electricity Costs (€)	3 513 440,85 €	3 402 076,97 €	3 292 436,81 €	3 182 796,65 €	3 073 156,49 €	2 963 516,33 €	2 853 876,17 €	2 744 236,01 €	2 634 595,85 €	2 524 955,69 €	2 415 315,53 €	2 305 675,37 €	2 196 035,21 €	2 086 395,05 €	1 976 754,89 €	1 867 114,73 €	1 757 474,57 €
	Cash-Flow (€)	(23 167,56) €	(61 804,67) €	(102 165,49) €	(142 526,32) €	(182 887,14) €	(223 247,96) €	(263 608,79) €	(303 969,61) €	(344 330,44) €	(384 691,26) €	(425 052,08) €	(315 411,92) €	(205 771,76) €	(96 131,60) €	13 508,56 €	123 148,72 €	232 788,88 €
0,5	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €	1,51 €	1,51 €	1,51 €	1,51 €			
	Revenues	4 500 029,52 €	4 312 528,29 €	4 125 027,06 €	3 937 525,83 €	3 750 024,60 €	3 562 523,37 €	3 375 022,14 €	3 187 520,91 €	3 000 019,68 €	2 812 518,45 €	2 625 017,22 €	2 625 017,22 €	2 625 017,22 €	2 625 017,22 €			
	Electricity Price (€/MW.h	57,30 €	55,48 €	53,69 €	51,90 €	50,12 €	48,33 €	46,54 €	44,75 €	42,96 €	41,18 €	39,39 €	37,60 €	35,81 €	34,02 €			
	Electricity Costs (€)	4 391 801,06 €	4 252 596,22 €	4 115 546,02 €	3 978 495,82 €	3 841 445,62 €	3 704 395,42 €	3 567 345,22 €	3 430 295,02 €	3 293 244,82 €	3 156 194,62 €	3 019 144,42 €	2 882 094,22 €	2 745 044,02 €	2 607 993,82 €			
	Cash-Flow (€)	(28 959,45) €	(77 255,83) €	(127 706,86) €	(178 157,89) €	(228 608,92) €	(279 059,95) €	(329 510,98) €	(379 962,01) €	(430 413,04) €	(480 864,07) €	(531 315,10) €	(394 264,90) €	(257 214,70) €	(120 164,50) €			
0,6	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €	1,51 €						
	Revenues	5 400 035,42 €	5 175 033,95 €	4 950 032,47 €	4 725 031,00 €	4 500 029,52 €	4 275 028,04 €	4 050 026,57 €	3 825 025,09 €	3 600 023,62 €	3 375 022,14 €	3 150 020,66 €						
	Electricity Price (€/MW.h	59,13 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €	44,85 €	43,06 €	41,28 €						
	Electricity Costs (€)	5 298 215,38 €	5 132 031,59 €	4 967 571,52 €	4 803 111,44 €	4 638 651,37 €	4 474 191,29 €	4 309 731,22 €	4 145 271,14 €	3 980 811,07 €	3 816 350,99 €	3 651 890,91 €						
	Cash-Flow (€)	(62 805,45) €	(121 623,14) €	(182 164,54) €	(242 705,94) €	(303 247,34) €	(363 788,74) €	(424 330,14) €	(484 871,54) €	(545 412,94) €	(605 954,34) €	(666 495,74) €						
0,7	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €							
	Revenues	6 300 041,33 €	6 037 539,61 €	5 775 037,88 €	5 512 536,16 €	5 250 034,44 €	4 987 532,72 €	4 725 031,00 €	4 462 529,27 €	4 200 027,55 €	3 937 525,83 €							
	Electricity Price (€/MW.h	59,13 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €	44,85 €	43,06 €							
	Electricity Costs (€)	6 204 578,15 €	6 011 417,01 €	5 819 548,64 €	5 627 680,28 €	5 435 811,92 €	5 243 943,56 €	5 052 075,20 €	4 860 206,84 €	4 668 338,48 €	4 476 470,12 €							
	Cash-Flow (€)	(96 599,89) €	(165 940,47) €	(236 573,83) €	(307 207,19) €	(377 840,55) €	(448 473,91) €	(519 107,28) €	(589 740,64) €	(660 374,00) €	(731 007,36) €							
0,8	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €								
	Revenues	7 200 047,23 €	6 900 045,26 €	6 600 043,30 €	6 300 041,33 €	6 000 039,36 €	5 700 037,39 €	5 400 035,42 €	5 100 033,46 €	4 800 031,49 €								
	Electricity Price (€/MW.h	59,13 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €	44,85 €								
	Electricity Costs (€)	7 111 060,18 €	6 890 918,01 €	6 671 637,69 €	6 452 357,37 €	6 233 077,05 €	6 013 796,73 €	5 794 516,41 €	5 575 236,09 €	5 355 955,77 €								
	Cash-Flow (€)	(130 513,60) €	(210 373,40) €	(291 095,04) €	(371 816,69) €	(452 538,34) €	(533 259,99) €	(613 981,64) €	(694 703,28) €	(775 424,93) €								
0,9	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €									
	Revenues	8 100 053,14 €	7 762 550,92 €	7 425 048,71 €	7 087 546,49 €	6 750 044,28 €	6 412 542,07 €	6 075 039,85 €	5 737 537,64 €									
	Electricity Price (€/MW.h	59,13 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €									
	Electricity Costs (€)	8 017 479,78 €	7 770 358,49 €	7 523 668,13 €	7 276 977,77 €	7 030 287,41 €	6 783 597,05 €	6 536 906,69 €	6 290 216,33 €									
	Cash-Flow (€)	(164 364,88) €	(254 745,80) €	(345 557,66) €	(436 369,51) €	(527 181,36) €	(617 993,22) €	(708 805,07) €	(799 616,93) €									
1	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €										
	Revenues	9 000 059,04 €	8 625 056,58 €	8 250 054,12 €	7 875 051,66 €	7 500 049,20 €	7 125 046,74 €	6 750 044,28 €										
	Electricity Price (€/MW.h	59,13 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €										
	Electricity Costs (€)	9 064 197,09 €	8 794 405,97 €	8 520 305,57 €	8 246 205,17 €	7 972 104,77 €	7 698 004,37 €	7 423 903,97 €										
	Cash-Flow (€)	(338 513,86) €	(443 725,21) €	(544 627,27) €	(645 529,33) €	(746 431,39) €	(847 333,45) €	(948 235,51) €										

Figure 24 - Print screen from FinancialAnalysis.xls (Silyzer 300 Cash flows at hydrogen selling price of 2.7 €/kg)

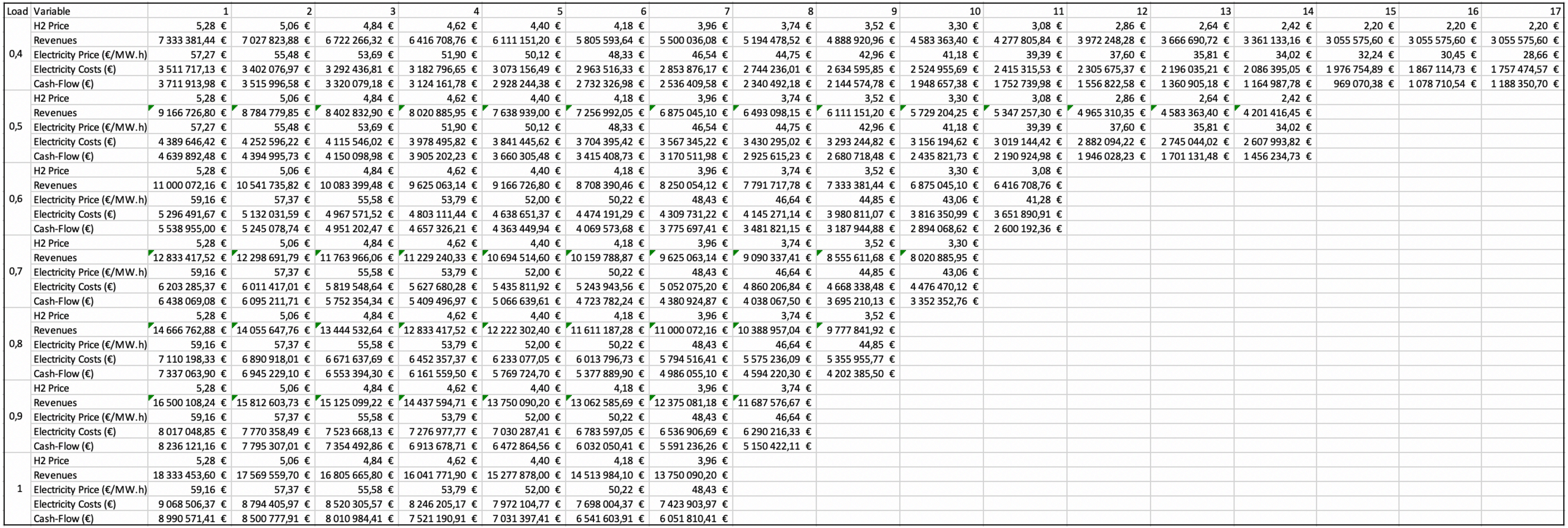
12 Appendix E – Thyssenkrupp’s 20 MW module Cash-flows (2.7 €·kg^{-1})



Load	Variable	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0,4	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €	1,51 €	1,51 €	1,51 €	1,51 €	1,51 €	1,51 €	1,51 €
	Revenues	4 468 525,06 €	4 282 336,51 €	4 096 147,97 €	3 909 959,42 €	3 723 770,88 €	3 537 582,34 €	3 351 393,79 €	3 165 205,25 €	2 979 016,70 €	2 792 828,16 €	2 606 639,62 €	2 606 639,62 €	2 606 639,62 €	2 606 639,62 €	2 606 639,62 €	2 606 639,62 €	2 606 639,62 €
	Electricity Price (€/MW.h)	64,94 €	62,89 €	60,87 €	58,85 €	56,82 €	54,80 €	52,78 €	50,75 €	48,73 €	46,71 €	44,69 €	42,66 €	40,64 €	38,62 €	36,59 €	34,57 €	32,55 €
	Electricity Costs (€)	4 551 134,90 €	4 407 405,44 €	4 265 645,93 €	4 123 886,43 €	3 982 126,92 €	3 840 367,41 €	3 698 607,91 €	3 556 848,40 €	3 415 088,90 €	3 273 329,39 €	3 131 569,88 €	2 989 810,38 €	2 848 050,87 €	2 706 291,37 €	2 564 531,86 €	2 422 772,35 €	2 281 012,85 €
	Cash-Flow (€)	(208 038,79) €	(250 497,87) €	(294 926,91) €	(339 355,95) €	(383 784,98) €	(428 214,02) €	(472 643,06) €	(517 072,10) €	(561 501,14) €	(605 930,17) €	(650 359,21) €	(508 599,71) €	(366 840,20) €	(225 080,70) €	(83 321,19) €	58 438,32 €	200 197,82 €
0,5	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €	1,51 €	1,51 €	1,51 €	1,51 €			
	Revenues	5 585 656,32 €	5 352 920,64 €	5 120 184,96 €	4 887 449,28 €	4 654 713,60 €	4 421 977,92 €	4 189 242,24 €	3 956 506,56 €	3 723 770,88 €	3 491 035,20 €	3 258 299,52 €	3 258 299,52 €	3 258 299,52 €	3 258 299,52 €			
	Electricity Price (€/MW.h)	64,94 €	62,89 €	60,87 €	58,85 €	56,82 €	54,80 €	52,78 €	50,75 €	48,73 €	46,71 €	44,69 €	42,66 €	40,64 €	38,62 €			
	Electricity Costs (€)	5 688 918,63 €	5 509 256,80 €	5 332 057,41 €	5 154 858,03 €	4 977 658,65 €	4 800 459,27 €	4 623 259,88 €	4 446 060,50 €	4 268 861,12 €	4 091 661,74 €	3 914 462,35 €	3 737 262,97 €	3 560 063,59 €	3 382 864,21 €			
	Cash-Flow (€)	(260 048,49) €	(313 122,34) €	(368 658,64) €	(424 194,93) €	(479 731,23) €	(535 267,53) €	(590 803,83) €	(646 340,12) €	(701 876,42) €	(757 412,72) €	(812 949,02) €	(635 749,63) €	(458 550,25) €	(281 350,87) €			
0,6	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €	1,51 €						
	Revenues	6 702 787,58 €	6 423 504,77 €	6 144 221,95 €	5 864 939,14 €	5 585 656,32 €	5 306 373,50 €	5 027 090,69 €	4 747 807,87 €	4 468 525,06 €	4 189 242,24 €	3 909 959,42 €						
	Electricity Price (€/MW.h)	66,77 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €	50,62 €	48,60 €	46,57 €						
	Electricity Costs (€)	6 858 763,39 €	6 644 154,39 €	6 431 515,34 €	6 218 876,30 €	6 006 237,25 €	5 793 598,20 €	5 580 959,16 €	5 368 320,11 €	5 155 681,06 €	4 943 042,02 €	4 730 402,97 €						
	Cash-Flow (€)	(344 119,23) €	(408 793,04) €	(475 436,81) €	(542 080,58) €	(608 724,35) €	(675 368,12) €	(742 011,89) €	(808 655,66) €	(875 299,43) €	(941 943,20) €	(1 008 586,97) €						
0,7	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €	1,62 €							
	Revenues	7 819 918,85 €	7 494 088,90 €	7 168 258,94 €	6 842 428,99 €	6 516 599,04 €	6 190 769,09 €	5 864 939,14 €	5 539 109,18 €	5 213 279,23 €	4 887 449,28 €							
	Electricity Price (€/MW.h)	66,77 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €	50,62 €	48,60 €							
	Electricity Costs (€)	8 028 541,46 €	7 778 987,34 €	7 530 910,69 €	7 282 834,04 €	7 034 757,38 €	6 786 680,73 €	6 538 604,07 €	6 290 527,42 €	6 042 450,76 €	5 794 374,11 €							
	Cash-Flow (€)	(428 123,27) €	(504 399,10) €	(582 152,40) €	(659 905,70) €	(737 659,00) €	(815 412,29) €	(893 165,59) €	(970 918,89) €	(1 048 672,18) €	(1 126 425,48) €							
0,8	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €	1,73 €								
	Revenues	8 937 050,11 €	8 564 673,02 €	8 192 295,94 €	7 819 918,85 €	7 447 541,76 €	7 075 164,67 €	6 702 787,58 €	6 330 410,50 €	5 958 033,41 €								
	Electricity Price (€/MW.h)	66,77 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €	50,62 €								
	Electricity Costs (€)	9 198 473,79 €	8 913 969,80 €	8 630 450,79 €	8 346 931,78 €	8 063 412,77 €	7 779 893,75 €	7 496 374,74 €	7 212 855,73 €	6 929 336,72 €								
	Cash-Flow (€)	(512 281,57) €	(600 154,67) €	(689 012,74) €	(777 870,82) €	(866 728,90) €	(955 586,97) €	(1 044 445,05) €	(1 133 303,12) €	(1 222 161,20) €								
0,9	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €	1,84 €									
	Revenues	10 054 181,38 €	9 635 257,15 €	9 216 332,93 €	8 797 408,70 €	8 378 484,48 €	7 959 560,26 €	7 540 636,03 €	7 121 711,81 €									
	Electricity Price (€/MW.h)	66,77 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €									
	Electricity Costs (€)	10 368 325,38 €	10 048 874,00 €	9 729 915,12 €	9 410 956,23 €	9 091 997,34 €	8 773 038,45 €	8 454 079,56 €	8 135 120,67 €									
	Cash-Flow (€)	(596 359,14) €	(695 831,98) €	(795 797,31) €	(895 762,65) €	(995 727,99) €	(1 095 693,32) €	(1 195 658,66) €	(1 295 623,99) €									
1	H2 Price	2,59 €	2,48 €	2,38 €	2,27 €	2,16 €	2,05 €	1,94 €										
	Revenues	11 171 312,64 €	10 705 841,28 €	10 240 369,92 €	9 774 898,56 €	9 309 427,20 €	8 843 955,84 €	8 378 484,48 €										
	Electricity Price (€/MW.h)	65,86 €	63,83 €	61,81 €	59,79 €	57,77 €	55,74 €	53,72 €										
	Electricity Costs (€)	11 538 177,24 €	11 183 778,47 €	10 829 379,71 €	10 474 980,94 €	10 120 582,18 €	9 766 183,41 €	9 411 784,65 €										
	Cash-Flow (€)	(680 436,96) €	(791 509,55) €	(902 582,15) €	(1 013 654,74) €	(1 124 727,34) €	(1 235 799,93) €	(1 346 872,53) €										

Figure 25 - Print screen from FinancialAnalysis.xls (Thyssenkrupp 20 MW model - Cash flows at hydrogen selling price of 2.7 €/kg)

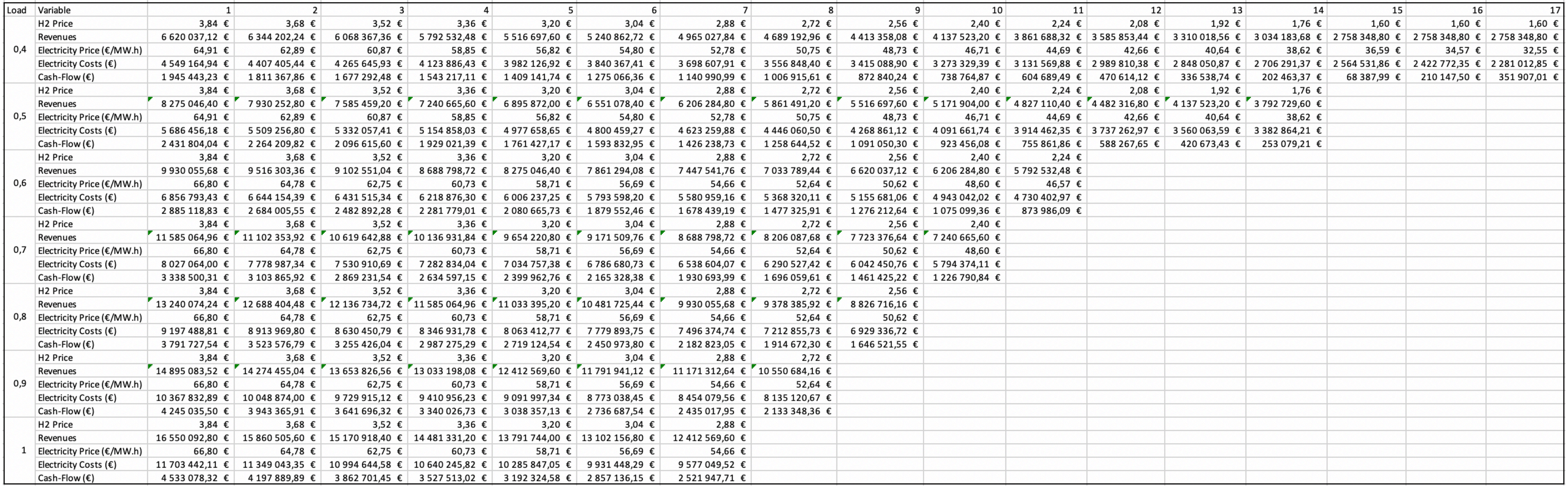
13 Appendix F – Silyzer 300 Cash-flows (5.5 €·kg^{-1})



Load	Variable	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0,4	H2 Price	5,28 €	5,06 €	4,84 €	4,62 €	4,40 €	4,18 €	3,96 €	3,74 €	3,52 €	3,30 €	3,08 €	2,86 €	2,64 €	2,42 €	2,20 €	2,20 €	2,20 €
	Revenues	7 333 381,44 €	7 027 823,88 €	6 722 266,32 €	6 416 708,76 €	6 111 151,20 €	5 805 593,64 €	5 500 036,08 €	5 194 478,52 €	4 888 920,96 €	4 583 363,40 €	4 277 805,84 €	3 972 248,28 €	3 666 690,72 €	3 361 133,16 €	3 055 575,60 €	3 055 575,60 €	3 055 575,60 €
	Electricity Price (€/MW.h)	57,27 €	55,48 €	53,69 €	51,90 €	50,12 €	48,33 €	46,54 €	44,75 €	42,96 €	41,18 €	39,39 €	37,60 €	35,81 €	34,02 €	32,24 €	30,45 €	28,66 €
	Electricity Costs (€)	3 511 717,13 €	3 402 076,97 €	3 292 436,81 €	3 182 796,65 €	3 073 156,49 €	2 963 516,33 €	2 853 876,17 €	2 744 236,01 €	2 634 595,85 €	2 524 955,69 €	2 415 315,53 €	2 305 675,37 €	2 196 035,21 €	2 086 395,05 €	1 976 754,89 €	1 867 114,73 €	1 757 474,57 €
	Cash-Flow (€)	3 711 913,98 €	3 515 996,58 €	3 320 079,18 €	3 124 161,78 €	2 928 244,38 €	2 732 326,98 €	2 536 409,58 €	2 340 492,18 €	2 144 574,78 €	1 948 657,38 €	1 752 739,98 €	1 556 822,58 €	1 360 905,18 €	1 164 987,78 €	969 070,38 €	1 078 710,54 €	1 188 350,70 €
0,5	H2 Price	5,28 €	5,06 €	4,84 €	4,62 €	4,40 €	4,18 €	3,96 €	3,74 €	3,52 €	3,30 €	3,08 €	2,86 €	2,64 €	2,42 €			
	Revenues	9 166 726,80 €	8 784 779,85 €	8 402 832,90 €	8 020 885,95 €	7 638 939,00 €	7 256 992,05 €	6 875 045,10 €	6 493 098,15 €	6 111 151,20 €	5 729 204,25 €	5 347 257,30 €	4 965 310,35 €	4 583 363,40 €	4 201 416,45 €			
	Electricity Price (€/MW.h)	57,27 €	55,48 €	53,69 €	51,90 €	50,12 €	48,33 €	46,54 €	44,75 €	42,96 €	41,18 €	39,39 €	37,60 €	35,81 €	34,02 €			
	Electricity Costs (€)	4 389 646,42 €	4 252 596,22 €	4 115 546,02 €	3 978 495,82 €	3 841 445,62 €	3 704 395,42 €	3 567 345,22 €	3 430 295,02 €	3 293 244,82 €	3 156 194,62 €	3 019 144,42 €	2 882 094,22 €	2 745 044,02 €	2 607 993,82 €			
	Cash-Flow (€)	4 639 892,48 €	4 394 995,73 €	4 150 098,98 €	3 905 202,23 €	3 660 305,48 €	3 415 408,73 €	3 170 511,98 €	2 925 615,23 €	2 680 718,48 €	2 435 821,73 €	2 190 924,98 €	1 946 028,23 €	1 701 131,48 €	1 456 234,73 €			
0,6	H2 Price	5,28 €	5,06 €	4,84 €	4,62 €	4,40 €	4,18 €	3,96 €	3,74 €	3,52 €	3,30 €	3,08 €						
	Revenues	11 000 072,16 €	10 541 735,82 €	10 083 399,48 €	9 625 063,14 €	9 166 726,80 €	8 708 390,46 €	8 250 054,12 €	7 791 717,78 €	7 333 381,44 €	6 875 045,10 €	6 416 708,76 €						
	Electricity Price (€/MW.h)	59,16 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €	44,85 €	43,06 €	41,28 €						
	Electricity Costs (€)	5 296 491,67 €	5 132 031,59 €	4 967 571,52 €	4 803 111,44 €	4 638 651,37 €	4 474 191,29 €	4 309 731,22 €	4 145 271,14 €	3 980 811,07 €	3 816 350,99 €	3 651 890,91 €						
	Cash-Flow (€)	5 538 955,00 €	5 245 078,74 €	4 951 202,47 €	4 657 326,21 €	4 363 449,94 €	4 069 573,68 €	3 775 697,41 €	3 481 821,15 €	3 187 944,88 €	2 894 068,62 €	2 600 192,36 €						
0,7	H2 Price	5,28 €	5,06 €	4,84 €	4,62 €	4,40 €	4,18 €	3,96 €	3,74 €	3,52 €	3,30 €							
	Revenues	12 833 417,52 €	12 298 691,79 €	11 763 966,06 €	11 229 240,33 €	10 694 514,60 €	10 159 788,87 €	9 625 063,14 €	9 090 337,41 €	8 555 611,68 €	8 020 885,95 €							
	Electricity Price (€/MW.h)	59,16 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €	44,85 €	43,06 €							
	Electricity Costs (€)	6 203 285,37 €	6 011 417,01 €	5 819 548,64 €	5 627 680,28 €	5 435 811,92 €	5 243 943,56 €	5 052 075,20 €	4 860 206,84 €	4 668 338,48 €	4 476 470,12 €							
	Cash-Flow (€)	6 438 069,08 €	6 095 211,71 €	5 752 354,34 €	5 409 496,97 €	5 066 639,61 €	4 723 782,24 €	4 380 924,87 €	4 038 067,50 €	3 695 210,13 €	3 352 352,76 €							
0,8	H2 Price	5,28 €	5,06 €	4,84 €	4,62 €	4,40 €	4,18 €	3,96 €	3,74 €	3,52 €								
	Revenues	14 666 762,88 €	14 055 647,76 €	13 444 532,64 €	12 833 417,52 €	12 222 302,40 €	11 611 187,28 €	11 000 072,16 €	10 388 957,04 €	9 777 841,92 €								
	Electricity Price (€/MW.h)	59,16 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €	44,85 €								
	Electricity Costs (€)	7 110 198,33 €	6 890 918,01 €	6 671 637,69 €	6 452 357,37 €	6 233 077,05 €	6 013 796,73 €	5 794 516,41 €	5 575 236,09 €	5 355 955,77 €								
	Cash-Flow (€)	7 337 063,90 €	6 945 229,10 €	6 553 394,30 €	6 161 559,50 €	5 769 724,70 €	5 377 889,90 €	4 986 055,10 €	4 594 220,30 €	4 202 385,50 €								
0,9	H2 Price	5,28 €	5,06 €	4,84 €	4,62 €	4,40 €	4,18 €	3,96 €	3,74 €									
	Revenues	16 500 108,24 €	15 812 603,73 €	15 125 099,22 €	14 437 594,71 €	13 750 090,20 €	13 062 585,69 €	12 375 081,18 €	11 687 576,67 €									
	Electricity Price (€/MW.h)	59,16 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €	46,64 €									
	Electricity Costs (€)	8 017 048,85 €	7 770 358,49 €	7 523 668,13 €	7 276 977,77 €	7 030 287,41 €	6 783 597,05 €	6 536 906,69 €	6 290 216,33 €									
	Cash-Flow (€)	8 236 121,16 €	7 795 307,01 €	7 354 492,86 €	6 913 678,71 €	6 472 864,56 €	6 032 050,41 €	5 591 236,26 €	5 150 422,11 €									
1	H2 Price	5,28 €	5,06 €	4,84 €	4,62 €	4,40 €	4,18 €	3,96 €										
	Revenues	18 333 453,60 €	17 569 559,70 €	16 805 665,80 €	16 041 771,90 €	15 277 878,00 €	14 513 984,10 €	13 750 090,20 €										
	Electricity Price (€/MW.h)	59,16 €	57,37 €	55,58 €	53,79 €	52,00 €	50,22 €	48,43 €										
	Electricity Costs (€)	9 068 506,37 €	8 794 405,97 €	8 520 305,57 €	8 246 205,17 €	7 972 104,77 €	7 698 004,37 €	7 423 903,97 €										
	Cash-Flow (€)	8 990 571,41 €	8 500 777,91 €	8 010 984,41 €	7 521 190,91 €	7 031 397,41 €	6 541 603,91 €	6 051 810,41 €										

Figure 26 - Print screen from FinancialAnalysis.xls (Silyzer 300 Cash flows at hydrogen selling price of 5.5 €/kg)

14 Appendix G – Thyssenkrupp’s 20 MW module Cash-flows (4 €·kg^{-1})



Load	Variable	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0,4	H2 Price	3,84 €	3,68 €	3,52 €	3,36 €	3,20 €	3,04 €	2,88 €	2,72 €	2,56 €	2,40 €	2,24 €	2,08 €	1,92 €	1,76 €	1,60 €	1,60 €	1,60 €
	Revenues	6 620 037,12 €	6 344 202,24 €	6 068 367,36 €	5 792 532,48 €	5 516 697,60 €	5 240 862,72 €	4 965 027,84 €	4 689 192,96 €	4 413 358,08 €	4 137 523,20 €	3 861 688,32 €	3 585 853,44 €	3 310 018,56 €	3 034 183,68 €	2 758 348,80 €	2 758 348,80 €	2 758 348,80 €
	Electricity Price (€/MW.h)	64,91 €	62,89 €	60,87 €	58,85 €	56,82 €	54,80 €	52,78 €	50,75 €	48,73 €	46,71 €	44,69 €	42,66 €	40,64 €	38,62 €	36,59 €	34,57 €	32,55 €
	Electricity Costs (€)	4 549 164,94 €	4 407 405,44 €	4 265 645,93 €	4 123 886,43 €	3 982 126,92 €	3 840 367,41 €	3 698 607,91 €	3 556 848,40 €	3 415 088,90 €	3 273 329,39 €	3 131 569,88 €	2 989 810,38 €	2 848 050,87 €	2 706 291,37 €	2 564 531,86 €	2 422 772,35 €	2 281 012,85 €
	Cash-Flow (€)	1 945 443,23 €	1 811 367,86 €	1 677 292,48 €	1 543 217,11 €	1 409 141,74 €	1 275 066,36 €	1 140 990,99 €	1 006 915,61 €	872 840,24 €	738 764,87 €	604 689,49 €	470 614,12 €	336 538,74 €	202 463,37 €	68 387,99 €	210 147,50 €	351 907,01 €
0,5	H2 Price	3,84 €	3,68 €	3,52 €	3,36 €	3,20 €	3,04 €	2,88 €	2,72 €	2,56 €	2,40 €	2,24 €	2,08 €	1,92 €	1,76 €			
	Revenues	8 275 046,40 €	7 930 252,80 €	7 585 459,20 €	7 240 665,60 €	6 895 872,00 €	6 551 078,40 €	6 206 284,80 €	5 861 491,20 €	5 516 697,60 €	5 171 904,00 €	4 827 110,40 €	4 482 316,80 €	4 137 523,20 €	3 792 729,60 €			
	Electricity Price (€/MW.h)	64,91 €	62,89 €	60,87 €	58,85 €	56,82 €	54,80 €	52,78 €	50,75 €	48,73 €	46,71 €	44,69 €	42,66 €	40,64 €	38,62 €			
	Electricity Costs (€)	5 686 456,18 €	5 509 256,80 €	5 332 057,41 €	5 154 858,03 €	4 977 658,65 €	4 800 459,27 €	4 623 259,88 €	4 446 060,50 €	4 268 861,12 €	4 091 661,74 €	3 914 462,35 €	3 737 262,97 €	3 560 063,59 €	3 382 864,21 €			
	Cash-Flow (€)	2 431 804,04 €	2 264 209,82 €	2 096 615,60 €	1 929 021,39 €	1 761 427,17 €	1 593 832,95 €	1 426 238,73 €	1 258 644,52 €	1 091 050,30 €	923 456,08 €	755 861,86 €	588 267,65 €	420 673,43 €	253 079,21 €			
0,6	H2 Price	3,84 €	3,68 €	3,52 €	3,36 €	3,20 €	3,04 €	2,88 €	2,72 €	2,56 €	2,40 €	2,24 €						
	Revenues	9 930 055,68 €	9 516 303,36 €	9 102 551,04 €	8 688 798,72 €	8 275 046,40 €	7 861 294,08 €	7 447 541,76 €	7 033 789,44 €	6 620 037,12 €	6 206 284,80 €	5 792 532,48 €						
	Electricity Price (€/MW.h)	66,80 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €	50,62 €	48,60 €	46,57 €						
	Electricity Costs (€)	6 856 793,43 €	6 644 154,39 €	6 431 515,34 €	6 218 876,30 €	6 006 237,25 €	5 793 598,20 €	5 580 959,16 €	5 368 320,11 €	5 155 681,06 €	4 943 042,02 €	4 730 402,97 €						
	Cash-Flow (€)	2 885 118,83 €	2 684 005,55 €	2 482 892,28 €	2 281 779,01 €	2 080 665,73 €	1 879 552,46 €	1 678 439,19 €	1 477 325,91 €	1 276 212,64 €	1 075 099,36 €	873 986,09 €						
0,7	H2 Price	3,84 €	3,68 €	3,52 €	3,36 €	3,20 €	3,04 €	2,88 €	2,72 €	2,56 €	2,40 €							
	Revenues	11 585 064,96 €	11 102 353,92 €	10 619 642,88 €	10 136 931,84 €	9 654 220,80 €	9 171 509,76 €	8 688 798,72 €	8 206 087,68 €	7 723 376,64 €	7 240 665,60 €							
	Electricity Price (€/MW.h)	66,80 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €	50,62 €	48,60 €							
	Electricity Costs (€)	8 027 064,00 €	7 778 987,34 €	7 530 910,69 €	7 282 834,04 €	7 034 757,38 €	6 786 680,73 €	6 538 604,07 €	6 290 527,42 €	6 042 450,76 €	5 794 374,11 €							
	Cash-Flow (€)	3 338 500,31 €	3 103 865,92 €	2 869 231,54 €	2 634 597,15 €	2 399 962,76 €	2 165 328,38 €	1 930 693,99 €	1 696 059,61 €	1 461 425,22 €	1 226 790,84 €							
0,8	H2 Price	3,84 €	3,68 €	3,52 €	3,36 €	3,20 €	3,04 €	2,88 €	2,72 €	2,56 €								
	Revenues	13 240 074,24 €	12 688 404,48 €	12 136 734,72 €	11 585 064,96 €	11 033 395,20 €	10 481 725,44 €	9 930 055,68 €	9 378 385,92 €	8 826 716,16 €								
	Electricity Price (€/MW.h)	66,80 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €	50,62 €								
	Electricity Costs (€)	9 197 488,81 €	8 913 969,80 €	8 630 450,79 €	8 346 931,78 €	8 063 412,77 €	7 779 893,75 €	7 496 374,74 €	7 212 855,73 €	6 929 336,72 €								
	Cash-Flow (€)	3 791 727,54 €	3 523 576,79 €	3 255 426,04 €	2 987 275,29 €	2 719 124,54 €	2 450 973,80 €	2 182 823,05 €	1 914 672,30 €	1 646 521,55 €								
0,9	H2 Price	3,84 €	3,68 €	3,52 €	3,36 €	3,20 €	3,04 €	2,88 €	2,72 €									
	Revenues	14 895 083,52 €	14 274 455,04 €	13 653 826,56 €	13 033 198,08 €	12 412 569,60 €	11 791 941,12 €	11 171 312,64 €	10 550 684,16 €									
	Electricity Price (€/MW.h)	66,80 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €	52,64 €									
	Electricity Costs (€)	10 367 832,89 €	10 048 874,00 €	9 729 915,12 €	9 410 956,23 €	9 091 997,34 €	8 773 038,45 €	8 454 079,56 €	8 135 120,67 €									
	Cash-Flow (€)	4 245 035,50 €	3 943 365,91 €	3 641 696,32 €	3 340 026,73 €	3 038 357,13 €	2 736 687,54 €	2 435 017,95 €	2 133 348,36 €									
1	H2 Price	3,84 €	3,68 €	3,52 €	3,36 €	3,20 €	3,04 €	2,88 €										
	Revenues	16 550 092,80 €	15 860 505,60 €	15 170 918,40 €	14 481 331,20 €	13 791 744,00 €	13 102 156,80 €	12 412 569,60 €										
	Electricity Price (€/MW.h)	66,80 €	64,78 €	62,75 €	60,73 €	58,71 €	56,69 €	54,66 €										
	Electricity Costs (€)	11 703 442,11 €	11 349 043,35 €	10 994 644,58 €	10 640 245,82 €	10 285 847,05 €	9 931 448,29 €	9 577 049,52 €										
	Cash-Flow (€)	4 533 078,32 €	4 197 889,89 €	3 862 701,45 €	3 527 513,02 €	3 192 324,58 €	2 857 136,15 €	2 521 947,71 €										

Figure 27 - Print screen from FinancialAnalysis.xls (Thyssenkrupp 20 MW model - Cash flows at hydrogen selling price of 2.7 €/kg)

15 Annex A - Silyzer 300 data sheet

siemens-energy.com

Silyzer 300

The next paradigm of PEM electrolysis

Large-scale industrial application
Silyzer 300 is the latest and most powerful product line in the double-digit megawatt class in the PEM electrolysis portfolio from Siemens.

Lowest investment costs
Silyzer 300's modular design makes unique use of scaling effects to minimize investment costs for large-scale industrial electrolysis plants. The optimized design results in very low hydrogen production costs thanks to high plant efficiency and availability.

Flexible and dynamic
Smart system solutions enable customer-specific, optimized configuration thanks to a high degree of design flexibility. The challenge of integrating renewable energy can be met by means of Silyzer 300's highly dynamic mode of operation.

Dependable service concept
We put together the perfect package for your individual needs. Our services range from basic maintenance activities to comprehensive all-round service using state-of-the-art data analysis.

Qualified partner
From grid integration to innovative instrumentation and controls, take advantage of the decades-long expertise and innovative strength of Siemens.

Proven technology
PEM electrolyzers in the Silyzer generation have proven themselves with our customers in the industrial, mobility, and energy sectors, and demonstrated their value in numerous in-house testing facilities. Our wealth of experience from decades of development and optimization has culminated in Silyzer 300.

Technical data

Hydrogen production:
100 – 2,000 kg per hour

Plant efficiency: > 75,5%

Startup time: < 1 minute

Dynamics: 0 – 100% in 10% / s

Minimum load: ≥ 5%

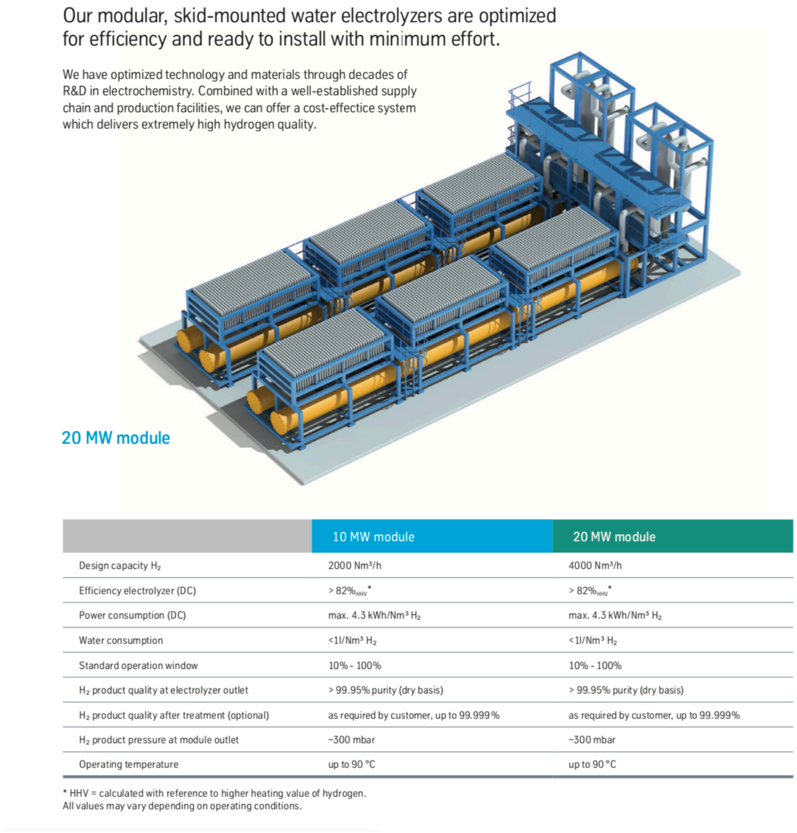
Water consumption (DI):
10 l per kg hydrogen

Hydrogen quality:
Ultra high purity 5.0

Silyzer 300 – PEM Module Array

Figure 29 - Silyzer 300 data sheet

16 Annex B - 20 MW Thyssenkrupp model data sheet



Our modular, skid-mounted water electrolyzers are optimized for efficiency and ready to install with minimum effort.

We have optimized technology and materials through decades of R&D in electrochemistry. Combined with a well-established supply chain and production facilities, we can offer a cost-effective system which delivers extremely high hydrogen quality.

20 MW module

	10 MW module	20 MW module
Design capacity H_2	2000 Nm^3/h	4000 Nm^3/h
Efficiency electrolyzer (DC)	> 82%$_{HHV}$*	> 82%$_{HHV}$*
Power consumption (DC)	max. 4.3 kWh/Nm^3 H_2	max. 4.3 kWh/Nm^3 H_2
Water consumption	<1l/Nm^3 H_2	<1l/Nm^3 H_2
Standard operation window	10% - 100%	10% - 100%
H_2 product quality at electrolyzer outlet	> 99.95% purity (dry basis)	> 99.95% purity (dry basis)
H_2 product quality after treatment (optional)	as required by customer, up to 99.999%	as required by customer, up to 99.999%
H_2 product pressure at module outlet	~300 mbar	~300 mbar
Operating temperature	up to 90 °C	up to 90 °C

* HHV = calculated with reference to higher heating value of hydrogen.
All values may vary depending on operating conditions.

Figure 30 - Thyssenkrupp's 20 MW model datasheet