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Optimization and Analysis of Power-To-Gas Technology Pathways

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Thesis to obtain the Master of Science Degree in

Energy Engineering and Management

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Abstract

In order to support the R&D activities in the field of power-to-gas, Fraunhofer ISE is developing a power-to-gas system simulator in the software environment (MATLAB, Simulink,Stateflow). The simulator enables stationary and dynamic system simulations based upon empirical characteristics as well as mass and energy balances of the most important components. In addition, a genetic optimization method has already been tested for the optimized dimensioning of central system components and control variables of the operation management or deployment strategy. Within the framework of the power-to-gas concept, the hydrogen pathway is considered while investigating PEM as electrolysis variant in the framework of Germany's energy system transition. With regard to the configuration of such systems, various scenarios are conceivable. Depending on the power source and the end application, they primarily differ in storage and distribution of the produced hydrogen. Taking into account the integration of such systems into inter-sectoral energy conversion chains, especially the integration of large amounts of wind energy makes up a challenging task. On the other site, building up a hydrogen supply infrastructure under current legal conditions and technology status is not challenging less. In order to improve the understanding of such systems under the constraints of integration possibilities into Germany's energy system, the aim of this thesis is to carry out diverse system simulations and optimizations for representative sites and chosen scenarios of dynamic operation with mainly wind energy.

Abstrato

Para apoiar as atividades R & D no campo do poder para o gs, o Fraunhofer ISE est desenvolvendo um simulador de sistema de energia para gs no ambiente de software (MATLAB, Simulink, Stateflow). O simulador permite simulaes de sistemas estacionrios e dinmicos com base em caractersticas empricas, bem como em balanas de massa e energia dos componentes mais importantes. Alm disso, um mtodo de otimizao gentica j foi testado para o dimensionamento otimizado de componentes do sistema central e variveis de controle do gerenciamento de operao ou estratgia de implantao. No quadro do conceito de energia para gs, a via de hidrogłnio considerada ao investigar a PEM como variante de eletrlise no quadro da transio do sistema energtico da Alemanha. No que diz respeito configurao de tais sistemas, vrios cenrios so concebveis. Dependendo da fonte de energia e do aplicativo final, eles diferem principalmente no armazenamento e na distribuio do hidrogłnio produzido. Levando em considerao a integrao de tais sistemas em cadeias de converso de energia intersetoriais, especialmente a integrao de grandes quantidades de energia elica constitui uma tarefa desafiadora. No outro site, a construo de uma infra-estrutura de fornecimento de hidrogłnio sob as atuais condies legais e status da tecnologia no um desafio menos. A fim de melhorar a compreenso de tais sistemas sob as restries das possibilidades de integrao no sistema de energia da Alemanha, o objetivo desta tese realizar diversas simulaes de sistemas e otimizaes para locais representativos e cenrios escolhidos de operao dinmica com principalmente energia elica.

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List of Symbols

Symbol	Description	Unit
ΔH_R	Enthalpy of Reaction	kJ mol^{-1}
G_R	Gibbs free Energy	kJ mol^{-1}
S_R	Entropy of reaction	kJ mol^{-1} K^{-1}
T	Temperature	K
V_{rev}	Reversible cell voltage	V
V_{th}	Thermoneutral cell voltage	V
F	Faraday Constant	C mol^{-1}
R	Gas Constant	C mol^{-1}
η_v	Voltage efficiency	-
η_F	Faraday efficiency	-
P_{tot}	Total Power of electrolyser	W
P_{nom}	Nominal Power of electrolyser	W
$V_{storage}$	Volume of storage tanks	m^3

List of Abbreviations / Acronyms

Abbreviation	Description
ASR	Area Specific Resistance
BoP	Balance of Plant
CAES	Compressed Air Energy Storage
CGH_2	Compressed Gaseous Hydrogen
DC	Direct Current
EEG	Erneuerbare-Energien-Gesetz
EEX	European Energy Exchange, Leipzig
EPEX SPOT	European Energy Exchange, Paris
EREC	European Renewable Energy Council
EU	European Union
FCV	Fuel Cell Vehicles
Grünanteil	Green Share
KPI	Key Performance Indicator
LCOE	Levelised Cost of Energy
LH_2	Liquid Hydrogen
MEA	Membrane Electrode Assembly
P2G	Power to Gas
PC	Price Cap
PEM	Proton Exchange Membrane
PHS	Pumped Hydro Storage
PS	Price Signal
PV	Photovoltaic
RES	Renewable Energy Sector
RVDF	Residual Value Distribution Factor
SOEC	Solid Oxide Electrolysis Cell
SOE	Solid Oxide Electrolyser
TES	Thermal Energy Storage
VLS	Full Load Hours
VLSpeicherzyklen	Full load storage cycles
Windanteil	Wind Share

1 Introduction

As a part of EU's "20-20-20 goals", The European Renewable Energy council(EREC) decided that by the year 2020, 20% of EU's energy on the basis of consumption must come from renewables. Figure 1 shows us the projections for the 2020 with respect to this goal. It can be seen that EU will meet it's target set by the EREC.

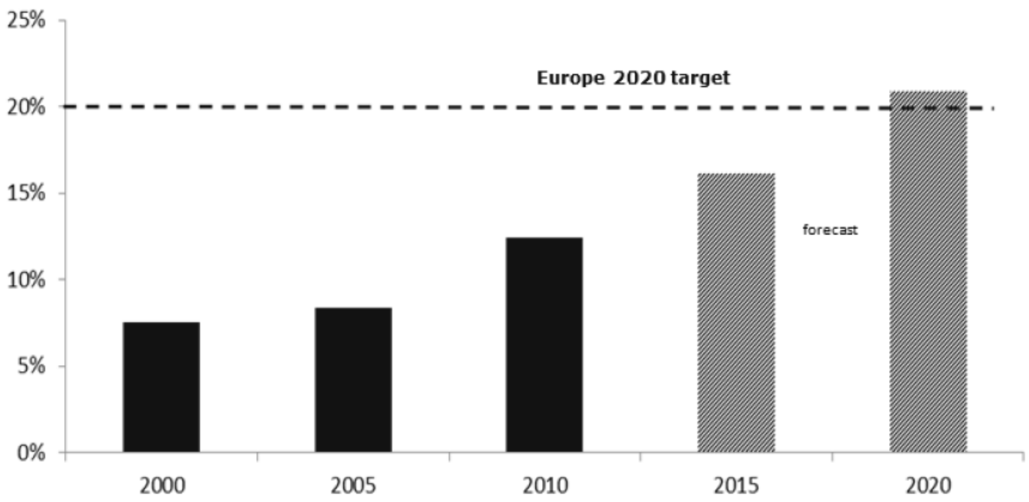


Figure 1: EU 20-20-20 Progress [1]

Member states of the EU believe that by 2020, 20.7% of renewable energy share will be achieved. On the other hand Renewable Energy Sector (RES) believes that a renewable energy share of 24.4% can be reached by 2020. 25 of the 27 member states of the EU are expected to reach their targets of which 16 member states are advancing in the direction that would help them surpass their targets. Also the member states predict that 11.27% of diesel and gasoline consumption in 2020 will be the share of renewables in transport sector.

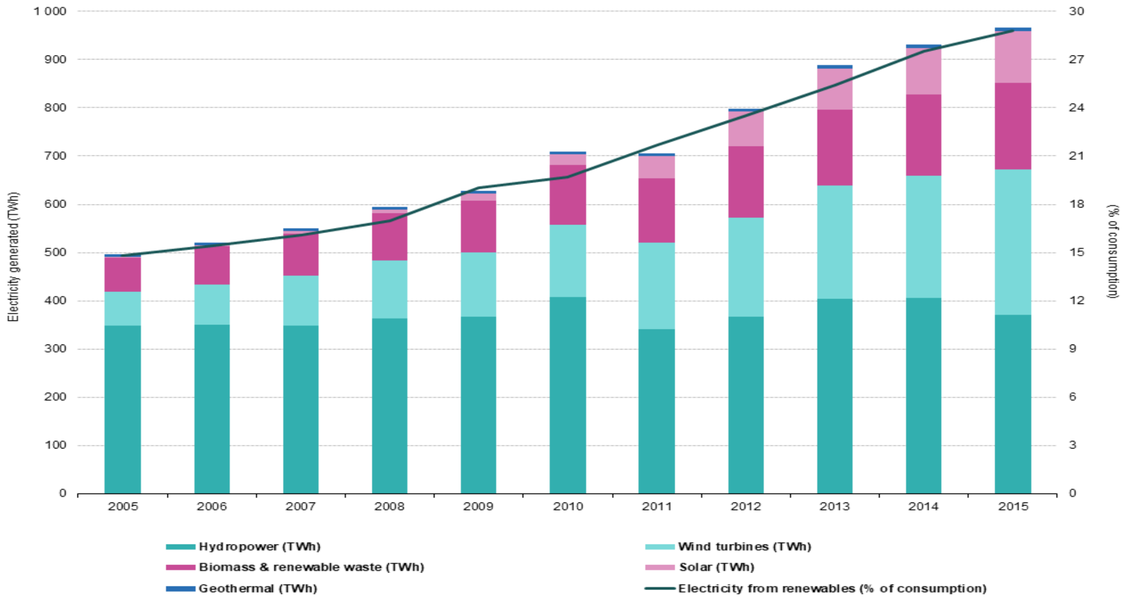


Figure 2: Annual Renewables split-up [2]

Figure 2 shows the growth of different types of renwables in the years from 2005 to 2015 [3]. It can be seen that wind and solar power share has considerably increased. Various studies and forecasts predict that this trend will continue for the next few years.

With increasing share of renwables, namely solar and wind in the grid, more erratic patterns of power production can be observed. This is due to the nature of renewable energy technolgies and emphasis the need for more reliable and high capacity energy storage technologies which ensure an energy supply throughout the year. There are various methods of energy storage. These methods are characterised by factors such a energy density, efficiency, location and or costs [4]. Chemical energy storage through batteries, mechanical energy storage techniques like pumped hydro storage(PHS), compressed air energy storage (CAES) and thermal energy storage (TES) like sensible TES, chemical TES, etc. are some methods. Each have their advantages and disadvantages. These have been summarised in table 1.

Method	**Advantages**	**Disadvantages**
Chemical Energy Storage	High efficiency	Low energy density
Mechanical Energy Storage	Mature technology, High energy and power capacity, long life	Requires special sites, high capital costs, long construction times
Sensible TES	Maximum temperature range of 400°C with concrete storage, low cost	Large size, good insulation is necessary to avoid increased heat losses with time
Chemical TES	High storage densities, low heat losses, compact	high capital costs, complex technology still in pilot project tests

Table 1: Advantages and disadvantages of various energy storage methods

Batteries due to their low capital costs and high efficiency are generally considered as the best short-term storage solution [5]. Their low energy density and high self-discharging rate makes them not suitable for long-term energy storage. Power-to-Gas(P2G) offers a very flexible way of controlling stochastic energy generation by renewables by producing hydrogen. Basically, hydrogen storage system has no self-discharging and the life cycle of such a system is estimated to be around 20,000 cycles and 15 years [6] due to which, hydrogen is considered to be a highly feasible energy storage solution for storage of excess electricity produced in the renewable energy sector. Also due to their nature of design, large plants of 100 MWh capacity and 10 MW peak load can be acheived [6]. It was estimated by Energy Technology Perspectives in 2012 that almost 14% of the electricity produced in 2050 will be used to produce hypdrogen [7].Production of Hydrogen can be done from natural gas, coal, hydrocarbons, biomass and also from water by water splitting. There are many methods to produce hydrogen, but electrolysis is one of the highly mature technology where electricity is be used to produce hydrogen. Electrolysis is the electrochemical process where water is split into hydrogen(H_2)and oxygen(O_2). This process is completely pollution free. There are many types of electrolysis process with advantages and disadvantages of their own. Alkaline water electrolysis is the most common method of water electrolysis with Proton Exchange Membrane(PEM) gaining popularity in recent times.

Power to gas (P2G) provides a very dynamic storage option, where the conventional storage options are not feasible or not enough. The main focus of this thesis is identifying suitable pathways depending upon the end usage and simulating real life scenarios for a year. At the end of the simulation, the LCOE of the pathway is determined and together with parameters like investment cost of the electrolysers and other components, impact of duties and taxes, lifetime of components, etc. gives a picture of how economically viable the pathway can be.

For doing this, MATLAB is primarily used in combination with simulink and state flow. Simulink and state flow facilitates the use of charts and and graphical medium eliminating the need for text based programming. There are various methods of optimization that can be used depending on the specific problem in question. Static or dynamic, discrete or continuous and Deterministic or stochastic are some examples. The choosing of a suitable optimization method is highly critical for obtaining accurate results. These are discussed in detail in section 5. Here a stochastic evolutionary algorithm will be used to do the optimization. This is used in combination with a parallel computing toolbox. The parallel computing tool box allows us to use the full power of multicore desktops and helps handling of data-intensive calculations smoothly [8].

The next few sections will deal basics of electrolysis and will focus on PEM technology to facilitate better understanding of the technology and the process.

2 Basics of Electrolysis

The simplest case of an electrolysis cell is shown in figure 3. A Direct Current(DC) power source is connected to the electrodes, which are plates here. Usually the plates are made from some inert materials and the process starts once the applied voltage is greater than the thermodynamic reversible potential.

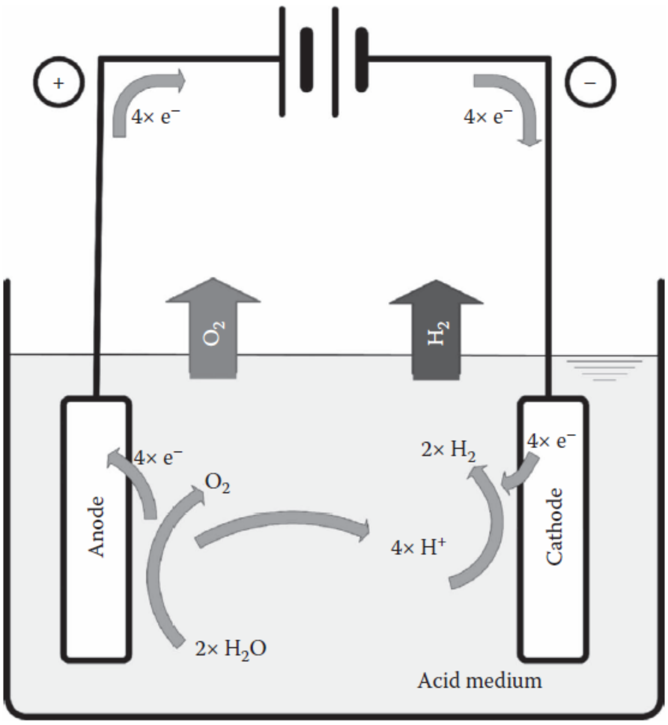


Figure 3: Priciple of water electrolysis cell with acid medium [9]

The basic principle of water electrolysis can be understood by equation that follows:

$$H_2O_{\,(l)} + \Delta H_R \longrightarrow H_{2(g)} + O_{2(g)} \tag{1}$$

The reaction shown in equation 1 is endothermic and ΔH_R is the change in enthalpy for that reaction. Since the reaction is endothermic, constant energy has to be supplied for the reaction to take place. Also the equation 1 shows the overall reaction in the electrolysis, whereas, there are oxidation and reduction reactions going on at the anode and cathode respectively. The electrochemical half reactions are shown below:

$$H_2O_{\,(l)} \longrightarrow \frac{1}{2}O_{2(g)} + 2\,H^+ + 2\,e^- \tag{2}$$

$$2\,H^+ + 2\,e^- \longrightarrow H_{2(g)} \tag{3}$$

Acid medium(electrolyte) is used for the process due to the limited self-ionization potential of

water. Also, since the ΔH_R for the reaction is negative(endothermic), a voltage greater than the thermoneutral voltage has to be supplied to operate a PEM electrolytic cell.
At the anode, the water is oxidised to produce oxygen, 2 protons and 2 electrons (equation 2). The electrons produced, migrate to the cathode via the external connection. The protons produced move through the electrolyte towards the cathode where it combines with the electrons from the external circuit to form hydrogen gas.
This process is clean, simple and easy to maintain. 99.999 % pure by volume hydrogen is obtained by this process [10]. The efficiency of the process is estimated to be around 70 % [10].

2.1 Alkaline Water Electrolysis

Alkaline water electrolysis is the most mature technology today in water electrolysis. They are highly reliable and have a liftime of around 15 years. Their investment costs are between 1000 €/kW and 5000 €/kW [11]. In this method, an alkaline solution acts as the electrolyte.Usually aqueous solution of KOH is used as the electrolyte. NaCl and NaOH are other possible but less common solutions that are used as an electrolyte. Figure 4 shows the process in an alkaline water electrolysis.

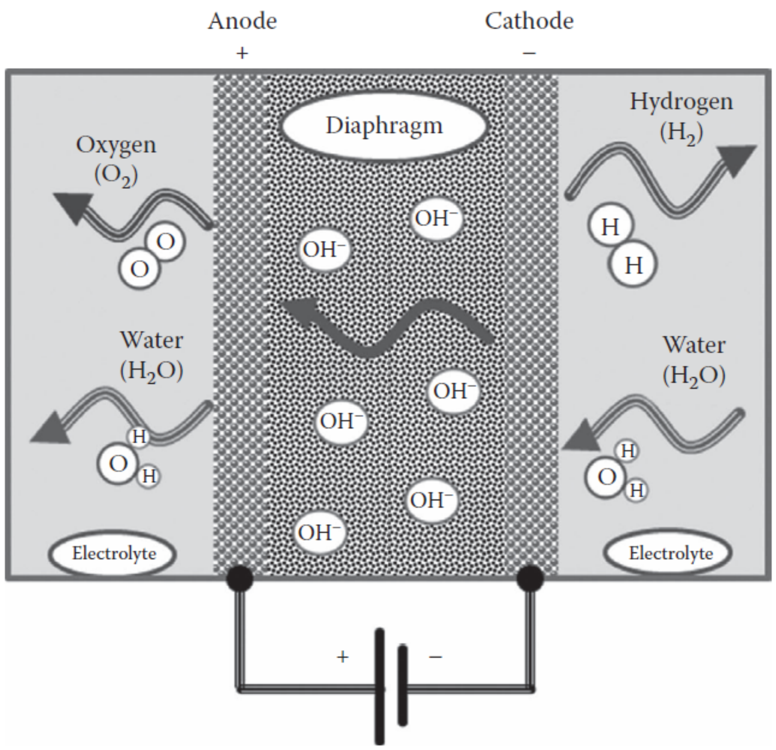


Figure 4: Alkaline Water Electrolysis [12]

Aqueous caustic solution of 20-30 % KOH is used as the electrolyte [13]. A diaphragm separates the electrodes. This keeps the product gases apart which in turn helps with the efficiency of the cell. During operation, at the cathode side, hydroxide anions produced by the reduc-

tion of water, travel through the electrolyte across the diaphragm to the surface of anode. At the anode they lose electrons and oxygen is produced . Also at the cathode side hydrogen is produced due to the reduction of water.
The electrochemical reactions at cathode and anode can be seen below:-

Cathode

$$H_2O + 2\,e^- \longrightarrow H_{2(g)} + 2\,OH^- \tag{4}$$

Anode

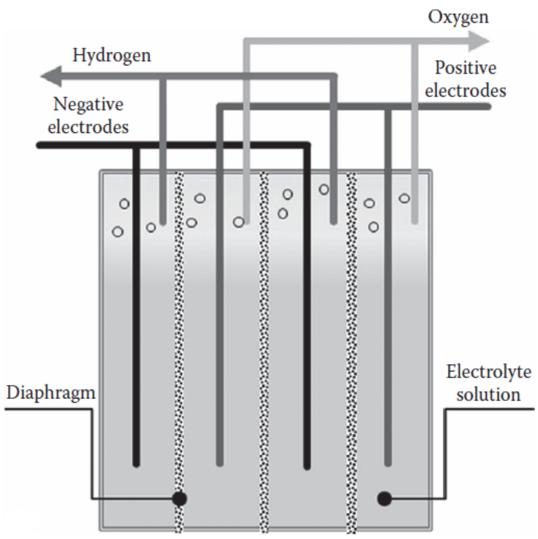
$$2\,OH^- \longrightarrow \frac{1}{2}\,O_{2(g)} + 2\,e^- \tag{5}$$

Overall

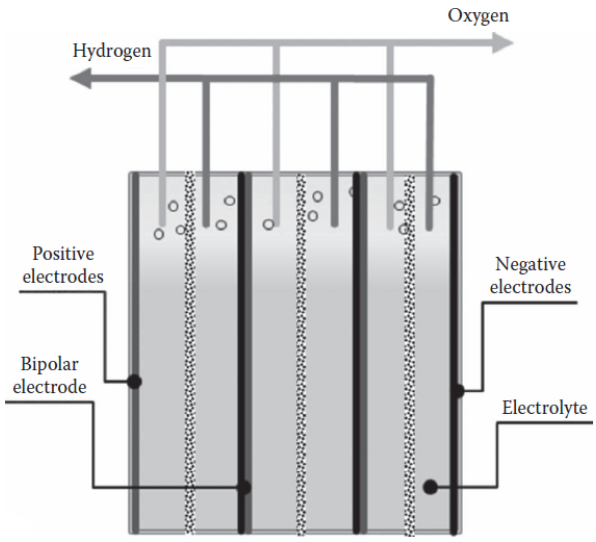
$$H_2O \longrightarrow H_{2(g)} + \frac{1}{2}O_{2(g)} \tag{6}$$

Hydrogen and oxygen gases produced at the cathode and anode respectively affects the cell resistance and decreases the contact area between the electrodes and electrolyte. Hence care has to be taken while designing the electrodes. The electrodes are usually of porous nature as this facilitates increased contact area between electrolyte and itself.

Low current density and highly corrosive environment are some of the drawbacks of this technology. Also the production rate is limited to 25-100 % [12]. This is because, at low loads, the production rate of oxygen is very low which increases the concentration of hydrogen to dangerous levels. This phenomenon is high at at partial and low loads. Usual operating pressures are usually low and in between 25 and 30 bar [12].
There are two configurations which are used commercially, unipolar and bipolar. This can be seen in figure 5.



(a) Unipolar



(b) Bipolar

Figure 5: Alkanline Water Electrolysis stack arragements [12]

In a unipolar arrangement, the stacks are connected parallely. The voltage across the cell is same as the voltage across the stack. In this configuration, the whole stack need not be shut down if one cell has a problem. Hence maintenance and construction of this configuration is simpler. On the other hand, in bipolar arrangement, the cells are connected in series. The electrodes have two polarities. The advantage of this arrangement is that higher current densities can be achieved which helps to produce gas at a higher pressure. Also the design is more compact compared to a unipolar arrangement.

2.2 Proton Exchange Membrane(PEM) water electrolysis

The Proton Exchange Membrane(PEM) technology is based on a solid polymer electrolyte instead of a liquid electrolyte. This electrolyte separates the two half cells and is called the Proton Exchange Membrane or the Polymer Electrolyte Membrane(PEM). A basic single cell in a PEM water electrolysis stack can be seen in figure 6.

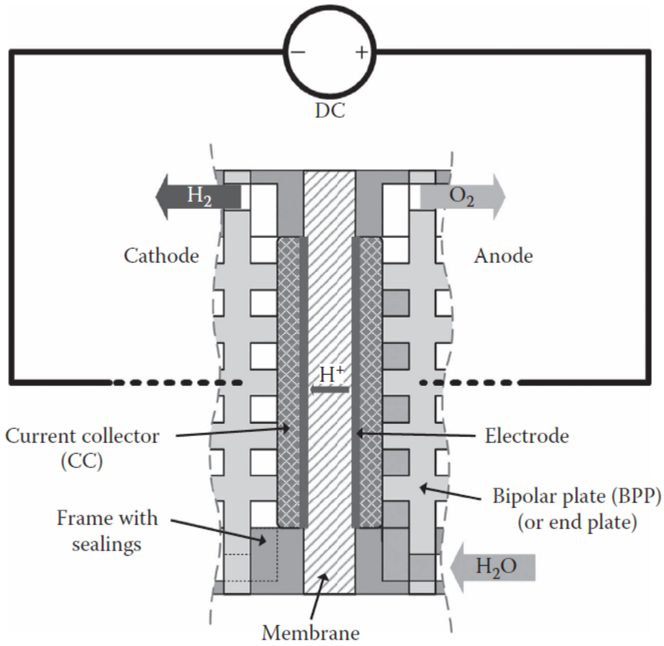


Figure 6: PEM water electrolysis stack [9]

The PEM is sandwiched between two the two electrodes. The electrodes also have the catalysts embedded in them and they are electrically insulated from each other. Also the electrodes instead of sandwiching the PEM, can also be deposited on either side of the PEM. This arrangement is commonly referred to as the Membrane Electrode Assembly (MEA). The bipolar plate or end plate provides a path for current to flow to the electrodes. The water is fed from the anode side and the H^+ ions produced travel through the polymer membrane to the cathode side. There is combines with electrons to produced hydrogen gas. The electrochemical half reactions are as follows:-

Cathode

$$2\,\mathrm{H}^+ + 2\,\mathrm{e}^- \longrightarrow \mathrm{H}_{2(g)} \tag{7}$$

Anode

$$\mathrm{H_2O} \longrightarrow \frac{1}{2}\,\mathrm{O}_{2(g)} + 2\,\mathrm{H}^+ + 2\,\mathrm{e}^- \tag{8}$$

Overall

$$\mathrm{H_2O} \longrightarrow \mathrm{H}_{2(\mathrm{g})} + \frac{1}{2}\mathrm{O}_{2(\mathrm{g})} \tag{9}$$

This design offers very good advantages over conventional designs. Some of them are as follows:-

- The main input apart from electricity is just pure water. This facilitates in maintaining a very simple design for the cell.
- The response time of the system is very high due to the compact size/design and its kinetic. This is a very important factor while considering the fact that this system will be interaction with renewable sources of energy whose output is very dynamic.
- The thin PEM layer is a shorter proton transfer path. This reduces the overall ohmic losses.
- The electro-catalysts have high efficiency and quick kinetics. This is because they are made from platinum group metals.
- The membrane helps to provide high gas tightness.

Similar to an alkaline water electrolysis cell, the cells are connected in parallel to for a stack. Higher hydrogen production rates can be achieved by this. The bipolar plates (BPP) separate adjacent cells. Thus the BPP acts as the cathode for one cell as well as the anode for the adjacent cell.

2.3 Solid Oxide Electrolysis

Solid Oxide Electrolysis is one of the methods of hydrogen production by electrolysis. As the name suggests, a solid electrolyte acts as the barrier between cathode and anode to prevent the hydrogen and oxygen produced from combining. Figure 7 shows a Solid Oxide Electrolysis Cell(SOEC).

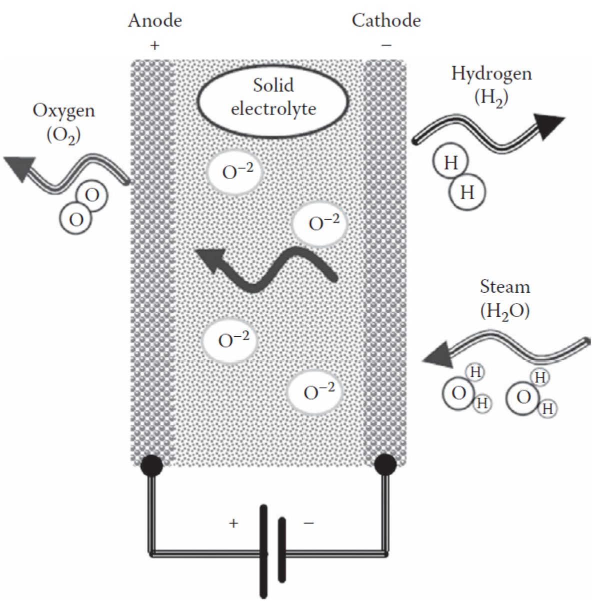


Figure 7: Solid Oxide Electrolysis Cell [12]

Steam or Carbon dioxide(CO_2) is electrochemically converted to hydrogen and carbon monoxide(CO). Steam or CO_2 is fed at the cathode side, where it is reduced and the resultant O^{-2} is transported to the anode side. Here, the O^{-2} combines with the electrons from the external circuit and oxygen is produced. The electrochemical reactions are shown below.

Cathode

$$\mathrm{H_2O + 2\,e^- \longrightarrow H_{2\,(g)} + O^{2-}} \tag{10}$$

$$\mathrm{CO_2 + 2\,e^- \longrightarrow CO + O^{2-}} \tag{11}$$

Anode

$$\mathrm{2\,O^{2-} \longrightarrow O_{2(g)} + 4\,e^-} \tag{12}$$

The solid electrolyte is arguably the most important part in this system and hence some criterion have to be met by it. High ionic conductivity, thermal and chemical stability are the preferred characteristics for a solid electrolyte. The most widely used material is yttria-stabilized zirconia(YSZ), while for anode, the most common materials are lanthanum, strontium, manganite (LSM).

The SOEs are usually operated at tempratures of range 873-1273 K [14]. This is because at low temperatures, the efficiency of a SOE is not satisfactory. Also, at high temperature, hydrogen can be produced at a much higher chemical reaction rate and there is low electric energy requirement [14]. Since the reaction here is endothermic and heat has to be supplied which tends to make the process less economical at higher temperature. Eventhough the electric energy demand decreases, there is an increase in demand for heat energy. The process becomes more economical if waste heat is supplied to supplement this increase in demand for heat [12].

It can be seen that each technology has it's own advantages and disadvantages. PEM with it's good response time, compact design and gas tightness is the main technology that is being used for the production of hydrogen. The next section with explain the PEM system and the kinetics of the cell.

3 PEM System

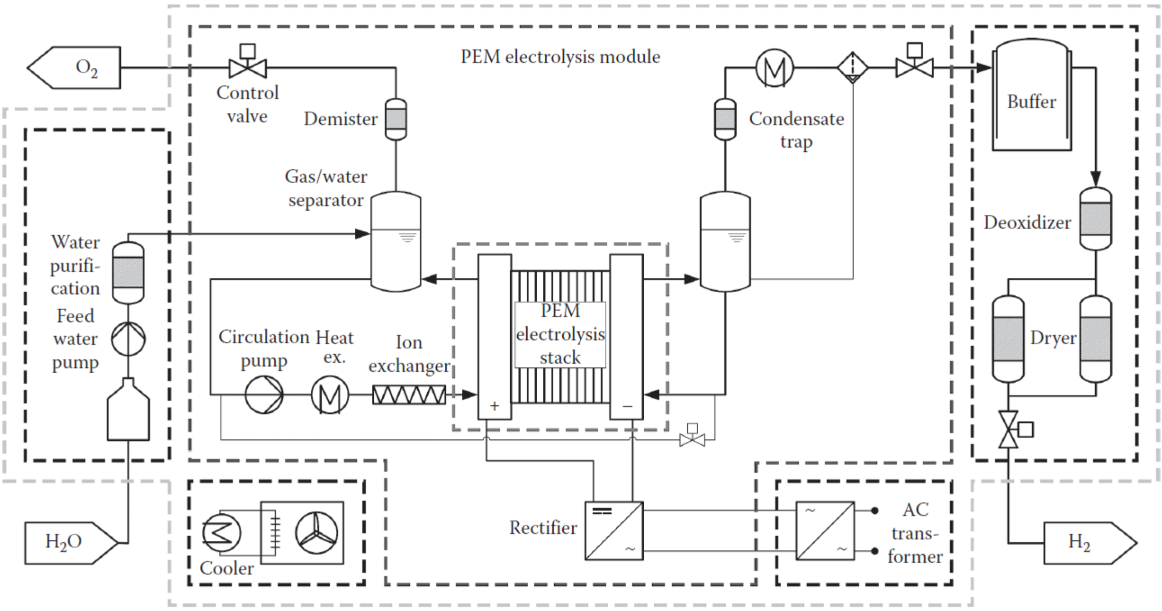


Figure 8: Basic layout of PEM System [9]

The basic layout of a PEM system is shown in figure 8. The PEM electrolysis stack is the heart of the system where the reaction takes place. All other peripheral systems are to make sure that the system operates in its optimum working conditions.

On the anode side there are components such as circulation pump, heat exchanger, ion exchanger, demister, gas/water separator and control valve.
The natural convection due to the rising gas is theoretically sufficient for the working of the system, but a dedicated circulation pump is important to ensure stack cooling. Also the feed water supply is connected to the anode side as this consumes water. Heavy metals can be trapped by the ion exchanger. The source of these metals may be from the Balance of Plant(BoP) or corrosion products. As the name suggests, a gas water separator separates the water that flows with the exiting gas. A demister is used to remove finer water droplets. The function of the control valve is to maintain the output pressure of the oxygen. The cathode side doesn't have a circulation pump. Water can also be observed in the cathode side as the electro-osmotic drag is sufficient to transport it from anode. Hence a smaller gas/water separator with a demister is used. A condensate trap is also used to reduce the dew point. The water collected is circulated back from the drain to the system.

On the system level, there are other subsystems that are installed based on the application. A buffer hydrogen tank is used to ensure smooth flow downstream of the system for it's application. Depending on the location of the system, the water quality might also vary. So a water purification system is also installed to maintain the quality of the water supplied. Also, the quality of hydrogen must be maintained to a great deal of accuracy depending upon the application. So hydrogen purification unit is also installed. Hydrogen and the remaining oxygen combines in the presence of a catalyst to form water. Then in the second stage, moisture is removed and the hydrogen is dried to the required dew point.

3.1 Thermodynamics of electrolysis

As mentioned earlier, since the decomposition of water is endothermic, the enthalpy of reaction(ΔH_R) has to be supplied. The standard enthalpy of reaction(ΔH_R) is 286 kJ mol^{-1} at standard temperature of $298K$ and standard pressure of 1.01325 Bar. The enthalpy of reaction can be shown as a function of Gibbs free energy(ΔG_R), temperature(T) and change in entropy of the reaction(ΔS_R) as shown in equation 13.

$$\Delta \mathrm{H_R} = \Delta \mathrm{G_R} + \mathrm{T} \cdot \Delta \mathrm{S_R} \tag{13}$$

Table 2 shows the values for change in enthalpy and change in entropy for the substances involved in equation 1 [15].

Substance(State)	ΔH_R (kJ mol^{-1})	ΔS_R(kJ/mol^{-1} K^{-1})
H_2O(l)	-285,83	69.942
O_2(g)	0	131.337
H_2(g)	0	205.817

Table 2: Enthalpy of Reaction and Change in entropy for water,oxygen and hydrogen

Based on the values from table 2, we get $\Delta G_R = 236.483$ KJ/mol. Assuming that there are no losses, the voltage across the electrodes is called the reversible cell voltage. With the Faraday constant(F) and number of moles of electrons involved in the reaction(n), the minimum voltage necessary to break down water can be calculated by equation 14.

$$V_{rev} = \frac{\Delta G_R}{n \cdot F} = 1.229V \tag{14}$$

where,
$n = 2$
$F = 96485$ C mol^{-1}

Without a heat source, the ΔH_R required for the reaction is also supplied electrically. This voltage is called the thermoneutral cell voltage(V_{th}). This can be calculated as shown in equation 15.

$$V_{th} = \frac{\Delta H_R}{n \cdot F} = 1.481V \tag{15}$$

Figure 9 shows the temperature dependance of thermal, electrical and total energy demand [15]. Until the point where phase transition takes place, it can be seen that the thermal energy demand increases whereas the electrical energy demand decreases. This results in a decrease of overall energy demand and hence justifies the preference to operate the stack at high temperatures.

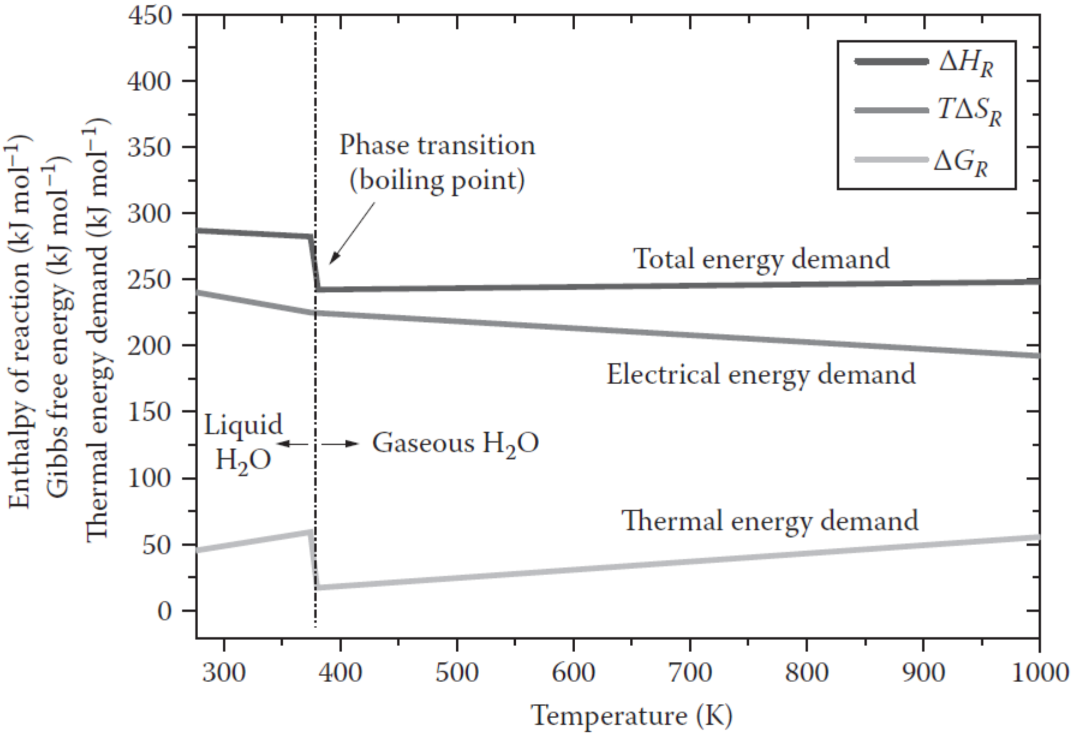


Figure 9: Temperature dependence of Thermal, Electrical and Total energy demand

It is also important to know that gibbs free energy and the enthalpy of reaction are not just dependant on the temperature but also pressure. Nernst equation gives us a function with reactant/product partial pressures and potential difference of the electrodes as shown below [9].

$$V_{rev} = V_{rev}^0 - \frac{R \cdot T}{2 \cdot F} \cdot \ln\left(\frac{a\{H_2O\}}{a\{H_2\} \cdot a\{O_2\}^{\frac{1}{2}}}\right) \tag{16}$$

Here, V_{rev}^0 is the reversible cell voltage calculated at STP in equation 14, R is the universal gas constant, F is the Faraday constant and $a\{H_2O\}, a\{H_2\}$ and $a\{O_2\}$ are the activities of reactants and products.

3.2 Electrolysis Kinetics

In reality, there are losses in the cell as the current flows through it. This causes the required cell voltage (V_{cell}) to be greater than its reversible cell voltage. These loses can be understood better by looking into the kinetics of electrolysis.

The losses in a cell can be broadly classified as faradaic and non-faradaic losses. Faradic losses occur during the transfer of electrons between the electrode and electrolyte. Faradaic losses occur due to the resistance to the flow of protons in the membrane and flow of electrons through cell components and electrodes. These losses are explained further in the next section.

3.2.1 Faradaic losses

As mentioned earlier, Faradaic losses occurs due to the mechanisms happening while there is a transfer of electrons between electrodes and electrolyte. Upon passing of current through the electrodes, there is a change from the state of thermodynamic equilibrium. This results in activation losses which are related to the rate of chemical reaction at the electrodes. By faraday's law, the amount of substance involved in the reaction and the amount of current transferred at the electrode can be related as follows:-

$$I = \frac{dQ}{dt} = z \cdot F \cdot \frac{dn}{dt} \tag{17}$$

where,

dn/dt is the rate of electrochemical reaction.

Since electrochemical reaction occurs on the surface, current density expressed in Acm^{-2} is a more accurate insight into the reality.

$$i = \frac{I}{A} \tag{18}$$

The net rate of chemical reaction can be calculated based on combining equations 17 and 19.

$$i = \frac{i}{z \cdot F \cdot A} = \frac{I}{z \cdot F} \tag{19}$$

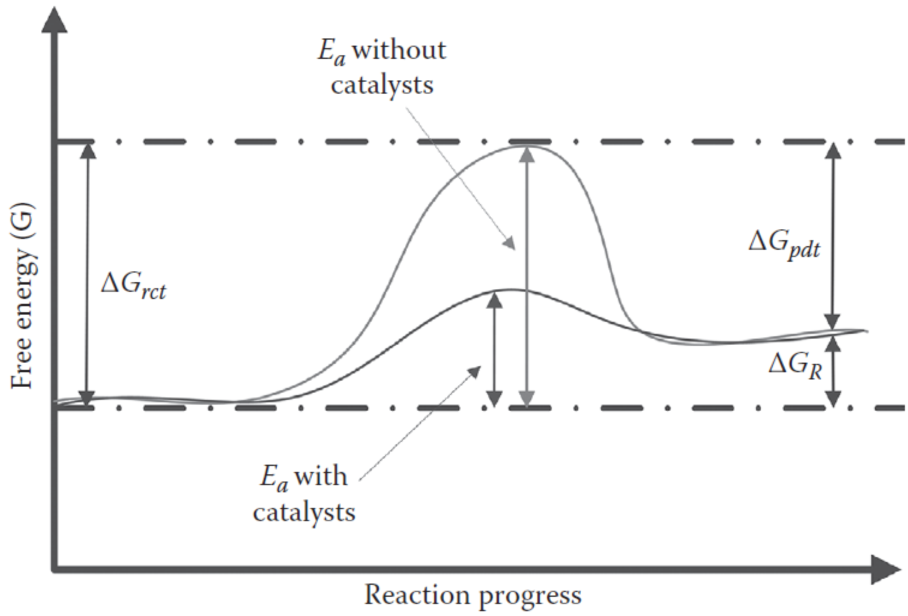


Figure 10: Activation energy vs reaction progress [9]

A certain activation energy (E_a) has to surpassed for the reaction to take place. This energy can be supplied as heat or as electric potential across the electrodes. The magnitude of this E_a can be varied by the use of catalysts. This is illustrated in figure 10.

3.2.2 Non-faradaic losses

Non-faradaic losses are the ones that occur due to the resistance offered to the flow of current by the components of the cell. As the reaction begins, there is a shift in thermodynamic equilibrium which naturally tends to slow down the rate of the reaction. This mechanism is governed by faraday's laws. It is assumed that the supply of reactants and removal of product from the reaction interface is not restricted. This makes the reaction faradaic in nature. However, this rate of transport influences the reaction kinetics as the equilibrium shifts.
The rate of the reaction is determined by the rate of supply of the reacting species. Also, since the reacting surface is porous and there are no more than two components reacting at both anode and cathode, Fick's diffusion is assumed to be the strongest transport mechanism.
Non-equilibrium electric potential of the reaction is given by the nernst equation:-

$$V = V^0 + \frac{R \cdot T}{n \cdot F} \cdot \ln(k) \tag{20}$$

Where,
k is the reaction rate constant at equilibrium and
$V - V^0 = \eta$ is the over potential
Assuming that c_i and c_b as the species concentration at the electrode interface and at a ref-

erence position respectively, we get $k = c_i/c_b$ and substituting this in equation 20 gives us :-

$$\eta_{con} = \frac{R \cdot T}{n \cdot F} \cdot \ln \left(\frac{c_i}{c_b} \right) \tag{21}$$

It can be seen from equation21 that the over potential is directly proportional to species concentration at reaction surface. Equation 21 has to be applied to cathode and anode separately. PEM electrolysers are operated at values of current density around 2 A cm^{-1}. At this range the product gases bubble which disrupts the contact between the electrode and electrolyte. The local current density increases due to this and this is quantified as bubbles over potential(η_{bub}). This increases with increasing current density exponentially (figure 11).

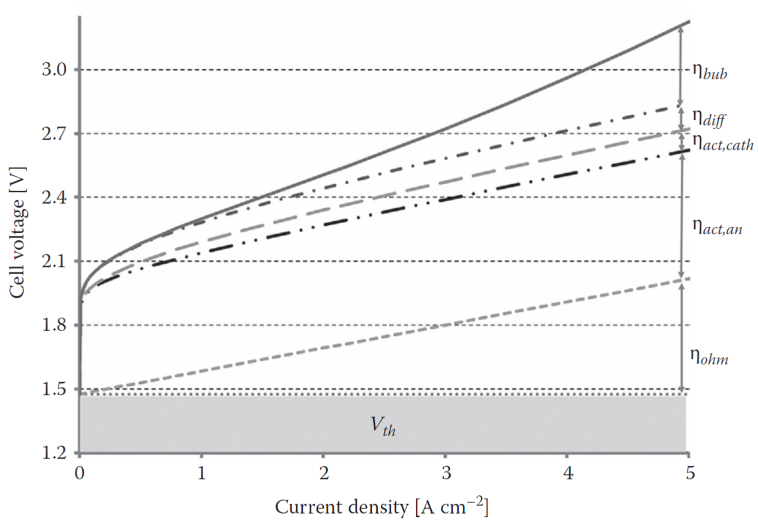


Figure 11: Overpotentials in a PEM cell [9]

Ohmic over potential (η_{ohm}) is another type of faradaic loss. Resistance to flow of electric current through cell components and proton movement through the membrane cause this over potential. It is given by:-

$$\eta_{ohm} = i \cdot ASR = \frac{I}{A} \cdot \sum R_i \tag{22}$$

ASR is the Area Specific Resistance which is the sum of all electrical and ohmic resistances.

3.3 Efficiency of PEM cell

There are more than one ways to calculate parameters that provides insight on the efficiency of the PEM cell. The voltage efficiency η_v can be expressed as shown in equation 23. This is used to judge the working of an electrolytic cell.

$$\eta_v = \frac{V_{th}}{V_{cell}} \tag{23}$$

The main purpose of the PEM electrolyser is the production of hydrogen. The amount of hydrogen produced ideally can be calculated using Faraday's law as shown in the equation below.

$$\dot{N}_{H_2,ideal} = \frac{I}{z \cdot F} \tag{24}$$

But it is known that there is loss of hydrogen produced due to diffusion through the solid membrane and this means that the amount of hydrogen actually produced($\dot{N}_{H_2,real}$) is lesser than that calculated in equation 24. This gives us the Faraday efficiency or loading efficiency.

$$\eta_F = \frac{\dot{N}_{H_2,real}}{\dot{N}_{H_2,ideal}} \tag{25}$$

The overall efficiency of the cell can be calculated using the voltage efficiency and the loading efficiency of the cell as shown in equation 26 [16].

$$\eta_{cell} = \eta_v \cdot \eta_F \tag{26}$$

3.4 Operation of PEM system

Availability of water at the electrode and a cell voltage higher than thermoneutral cell voltage at ambient temperature are the conditions that are necessary to operate a PEM electrolyser at atmospheric conditions. As most of the applications calls for hydrogen at pressure, electrolysers are operated under pressure. This also eliminates the necessity of a compressor to provide hydrogen at higher pressures. There are three common ways of PEM operations. They are listed below:-

- Differential or balanced pressure operation.
- Anode or cathode water feed operation.
- Thermal management by circulation of water at anode and cathode.

Each of these operation method calls for some changes in stack design for optimization. For example, for differential pressure type of operation, the hydrogen side works under high pressure. The oxygen side is slightly pressurised or not pressurised at all. So in this case, stacks have to be designed to withstand the pressure difference. In case of a balanced pressure operation, both the anode and cathode sides are operated under the same pressure.

In a water feed opertation, water can be fed on either cathode or anode side. As shown in figure 6, most of the PEM electrolysers are operated with anode water feed. Cathode water feed are also used in some special applications. Since water is consumed in the anode and not in the cathode, water has to move from the cathode to anode. This is a limitation which finally leads to a larger cell for same rates of hydrogen production [9].
Thermal management is realised by a dedicated circulation system with circulation pump, heat exchanger, gas/water separator and water supply. This can be see in figure 8.
These management methods, kinematics of the cells are all characterised in the model of the electrolyser used for simulation. This is accomplised with the help of the partners who produce the electrolyser and Fraunhofer.

4 Power to Gas

After a brief introduction into the dynamics of a PEM electroysis system and it's working, it is important to know where the PEM system stands with respect to the bigger scenario. Power to Gas (P2G)is a methodology that converts power to gaseous fuel [17]. This enables the intermittent production of energy by renewables to be evened out throughout the year by providing them a controllable power load and hence enabling them to have a bigger energy share. Also, de-carbonisation of gas sector, mobility sector and industrial sector is helped as renewable power is converted into a natural gas substitute. The simulation uses a system model and the components of this system is shown and explained in the next section.

4.1 System components

The schematic drawing of the system that is used here for the simulation is shown in figure 12[1,2].

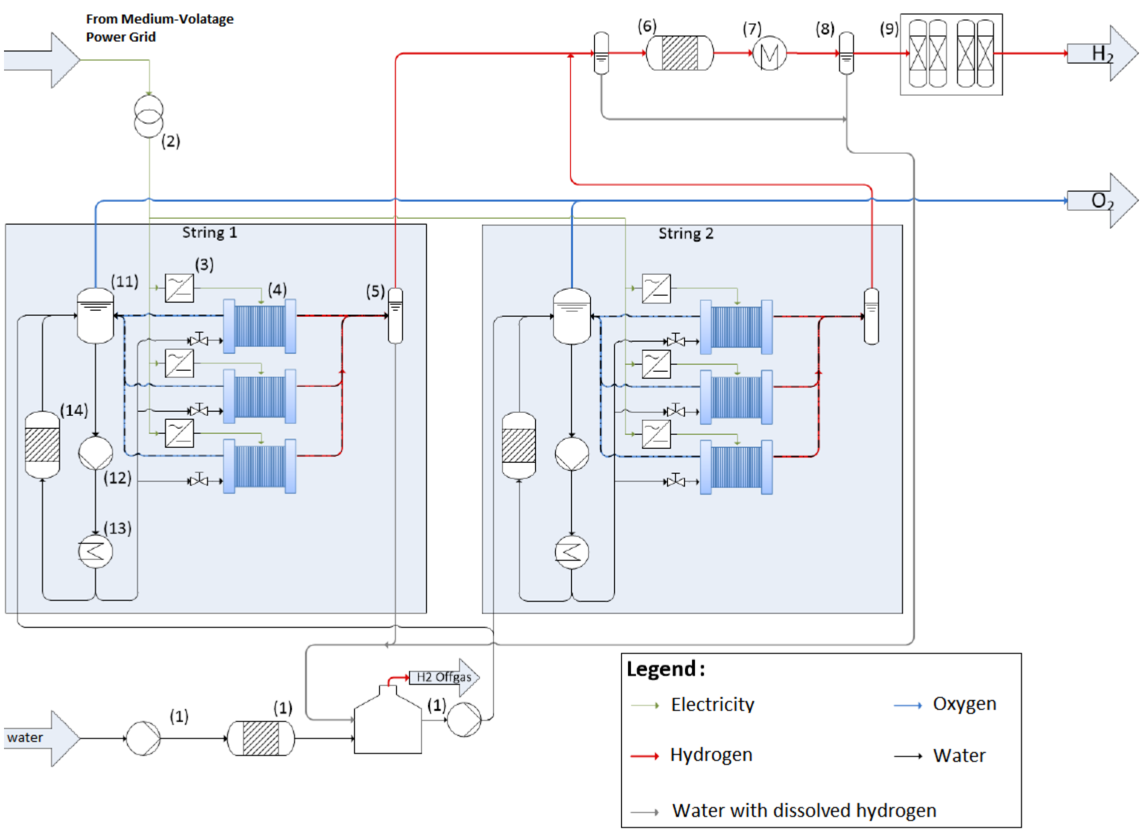


Figure 12: Schematic of the electrolysis sytem [18]

A string concept is used here. Strings are a set of stacks combined together. In the figure 12, it can be seen that 3 stacks make up the strings. It can be more depending upon the usage and

[1] Refer appendix A.3 for the component names shown in figure 12.
[2] Figure translated from German to English for better understanding

convenience of the designer. There are examples of 100 MW systems where the strings are composed of 10 stacks each [19]. This is an advantage because this technique reduces the number of auxilary components required. Also due to this, the model in the optimization is also simplified which helps with reducing the computaional times.

Based on what can be accomplished using P2G methodology, a large number of scenarios and pathways are possible. The following section looks further into the scenarios.

4.2 Pathways

The main catch here is that wind and photovoltaic are a very good source of energy but erratic. It is seen from the comparison between the past annual power generation and electricity demand that there is a mismatch. There can be more energy produced than the demand and vice-versa. With higher degrees of renewable technology energy share in electricity generation, there is a need for large storage systems. Power to gas provides a very dynamic method of putting to use this erratic power produced. Depending on the application of the produced hydrogen, the size, operating pressure and other parameters change.

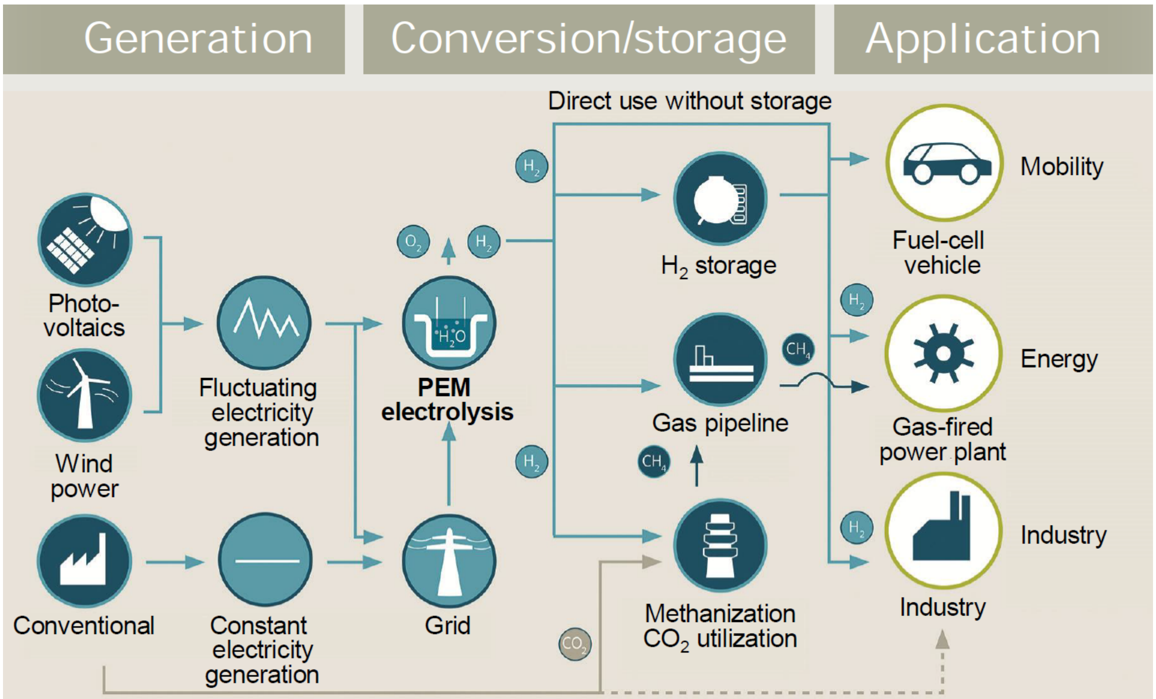


Figure 13: Pathways downstream and upstream of PEM system [20]

Figure 13, shows the general scenario and the possible pathways before and after the PEM system. It can be seen that the hydrogen produced through PEM can be stored in tanks. Also, they can be fed into the natural gas pipelines according to its asking norms. Storage of hydrogen is a very interesting scenario. This is because in this pathway, Power to Gas provides an opportunity to use hydrogen (fuel cells) as a fuel in transportation sector when high renewable penetration makes it less economical to use batteries [20].

4.3 Hydrogen Storage

Hydrogen storage is another interesting aspect in P2G technologies. With the rise of fuel cell cars, more emphasis is being laid on the importance of providing hydrogen at competitive prices for mobility sector. There are many ways of producing hydrogen, but P2G focusses on providing the hydrogen from renewable energy resources.
Since production of hydrogen considered here is based on wind power, right now it is costly, limited and hard to centralise. So one of the options would be to produce hydrogen close to the wind power plants which can be stored onsite in tanks. This can be then transported to the desired locations which would be the hydrogen refuelling stations. The economics of this type of arrangement will be dealt with in the results section of this thesis.Also there are various requirements that have to met by the hydrogen to be used in the mobility sector. These include fuel(H_2) quality, codes and standards that have been laid on the storage and usage of fuel cell vehicles(FCV). Also, Ford motor company did a study in USA and concluded that about 33% of the existing fuel stations should provide hydrogen refuelling options for a customer to consider buying a FCV that runs only on hydrogen [21].

4.4 Hydrogen and Natural Gas

It has been establised that upto 10 % by volume of hydrogen can be added to the natural gas gird without any effects. . But this doesn't ensure that the systems that use natural gas for their processess like gas turbines or auxilary systems like underground storage of natural gas will all work properly. Right now gas turbines can work with a hydrogen fraction of 1% by volume or lesser [22].
Various researches are being done to understand the limits to which hydrogen can be added to the natural gas grid. This involves comparing the properties of gas that are important to satisfy their primary objective. Wobbe index is one such property. Wobbe index is a value that denotes the interchangeability of gases. In simple terms, if two gases have the same wobbe index at same pressure and setting, then their energy output will be the same. Figure 14 shows the change in wobbe index for some gases on adding hydrogen.

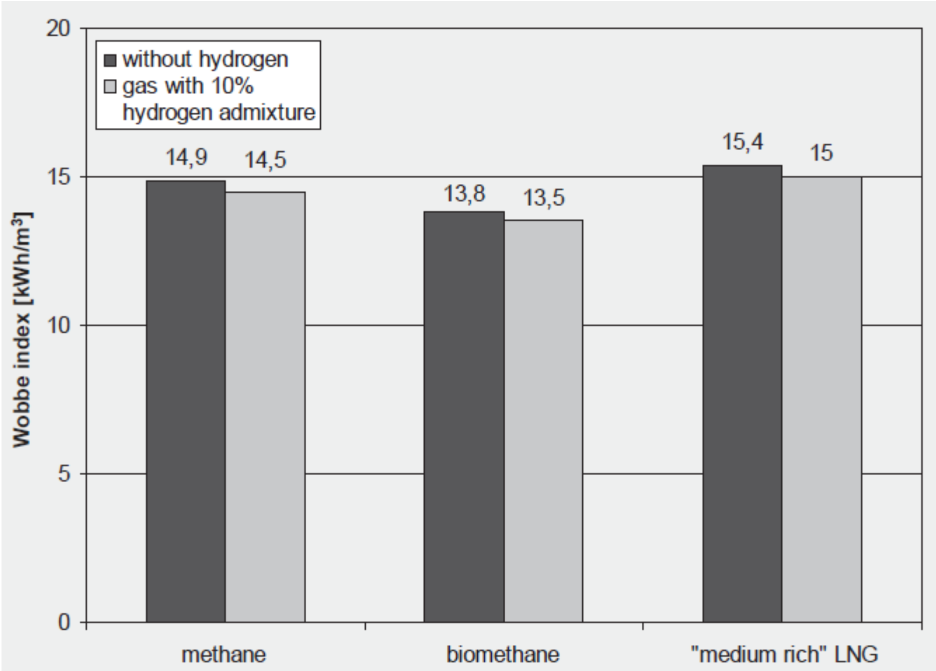


Figure 14: Change in Wobbe index due to addition of hydrogen [22]

Changes in other properties like methane number, laminar flame speed, etc. must be considered carefully. Also other factors like hydrogen embitterment, transmission and in house pipelines to be make leak proof for hydrogen, industrial applications, etc. all have to be proved to accept the permissible level of hydrogen in the natural gas pipelines.

4.5 Hydrogen filling and transportation

Storage of hydrogen is one of the major challenges. This depends on what is the usage of the produced hydrogen. Today, storage of hydrogen upto 1000 bar is possible [23]. Since the locations of wind farms are not centralised and this in turn makes the location P2G plants away from the demands. So produced hydrogen has to be transported in trailers as Compressed gaseous hydrogen(CGH_2) or liquid hydrogen(LH_2). CGH_2 is transported at pressures of 200 bar [23]. Pipelines transport hydrogen at 20-100 bar pressure range [23].

Various parameters have effect on the condition of the gas when filling. It can be seen from figure 15 that, increasing the rampup pressure leads to higher peak temperature. At lower rampup rates, the temperature seems to be fairly constant throughout time.

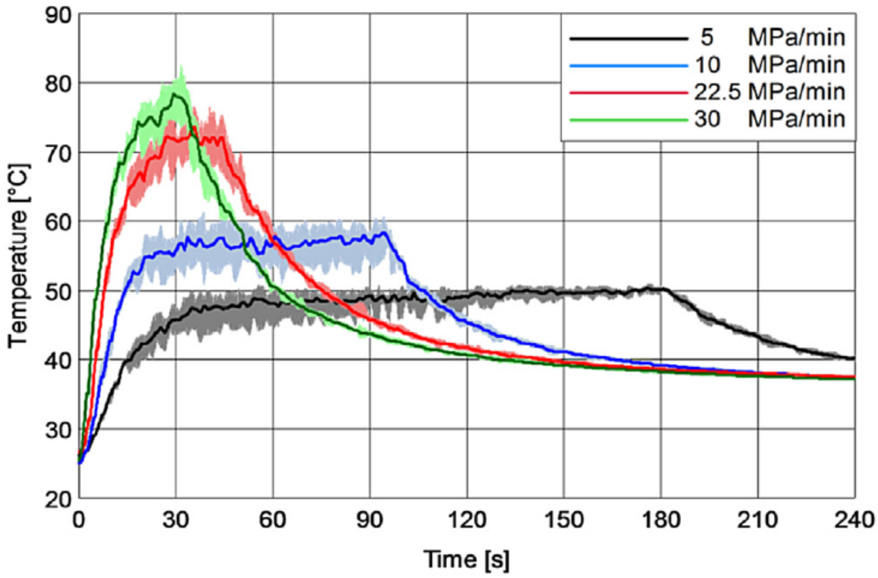
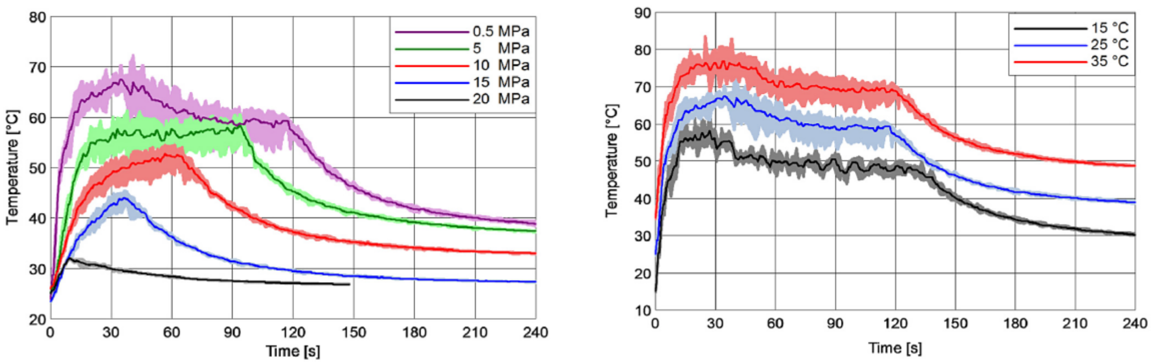


Figure 15: Gas temperature profile vs time for various pressure rampup rates [24]

Similarly, initial pressure, ambient temperature and initial temperature all affect the gas temperature profile over time. These effects are illustrated in the figures 16a and 16b



(a) Different initial pressures (b) Different ambient temperatures

Figure 16: Gas temperature profile vs time [24]

Due to these effects, above 10 bar, the ideal gas equations are not used calculations but the real gas equation according to Soave-Redlich-Kwong shown below is used.

$$P = \frac{R \cdot T}{V_m - b} - \frac{a \cdot \alpha(T)}{V_m \cdot (V_m + b)} \tag{27}$$

where,
P is the pressure,
V_m is the molar volume,
b is the co-volume,
T is the temperature,
a is the cohesion pressure and

$\alpha(T)$ is a dimensional factor (1 at critical temperature).

Now, the pathways that are going to be analysed are explained. Major analysis is done for pathways with different end users.

4.6 Path 1

Figure 21 shows the pathway being considered. This pathway focuses on the economics analysis of producing hydrogen from wind power mainly for mobility purposes. Fuel cell cars are gaining more attention today due to their low carbon footprint. This creates an interest in knowing how much the cost would be if a PEM electrolyser system is used produce hydrogen which are stored in tanks. This later is used to fill up fuel cell cars in hydrogen filling stations. The source of electricity used for this is mainly from wind power.

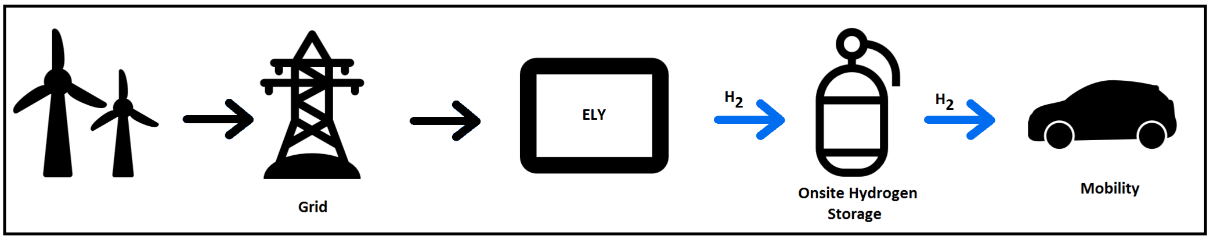


Figure 17: Path 1

There are various types of variable that are considered in this scenario. **Reference years** are one of the most important variable. The simulations are done for the years 2014, 2030 and 2050 to see how the prices of hydrogen produced by this pathway varies. Next variable would be the **cost of the electricity** that is used in the electrolyser for the production of hydrogen. The German Renewable Energy sources Act (Erneuerbare-Energien-Gesetz or EEG in german) was implemented to encourage production of energy from renewable resources. The EEG amounts to 62.4 €/MWh. This represents the full taxes scenario (table 3). A concession is given for consumption above 1GWh. Above 1GWh, the EEG is 1 €/MWh. This corresponds to the scenarios where the taxes are reduced.The pathway has various scenarios based on the variables for that specific pathway. This results in a scenario matrix that will tell us the combinations of variables that have been considered for each path way. The table 3 shows the resultant scenario matrix.

Scenario	Operation Strategy	Year	Taxes
1 2 3	Combined Price Arbitage	2014	Full Reduced Free
4 5 6	Combined Price Arbitage	2030	Full Reduced Free
7 8 9	Combined Price Arbitage	2050	Full Reduced Free
10 11 12	More than 50 % R.E. in the grid	2014	Full Reduced Free
13 14 15	More than 75 % R.E. in the grid	2030	Full Reduced Free
16 17 18	More than 95 % R.E. in the grid	2050	Full Reduced Free

Table 3: Scenario Matrix for Path 1

4.7 Path 2

Similar to path 1, path 2 also uses electricity from wind power predominantly. Figure 18 shows this pathway. Here, the produced hydrogen is stored in caverns underground before it is fed into the grid. Here it is interesting to note that today there is no dedicated hydrogen gas grid. Hence the existing natural gas grid is used for delivering hydrogen to the end user. Maybe in future, there will a necessity and a hydrogen gas grid might be created exclusively for this purpose. The end users in this pathway are the industries and mobility sector.

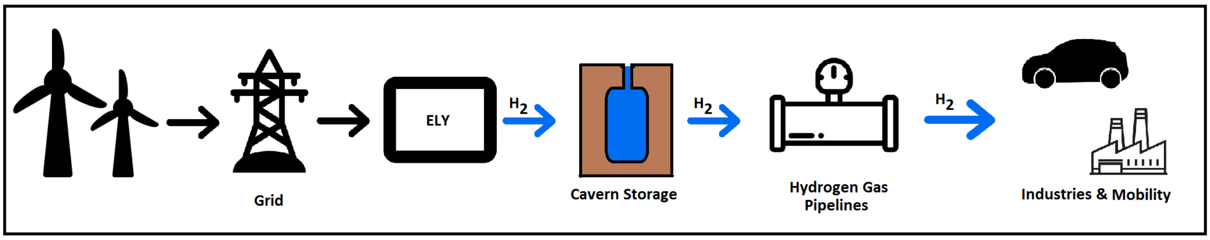


Figure 18: Path 3

In this scenario, the is an assumption that the renewable energy park can be constructed along with an electrolyser plant to satisfy the demand for hydrogen. In the first eight scenarios considered in this pathway, industry is the assumed end user.
Like in the previous pathway, there are different variables that contribute and result in a scenario matrix shown in table 4. The location for this pathway is chosen to be Berlin, the capital city of Germany. For the initial scenario, the possibility of a Renewable energy park with no size restriction close to an industry with constant demand of hydrogen is assumed. This eliminated the possibility of long hydrogen pipelines as the production is done at the place of usage. In the second scenario, a restriction on the size of wind and PV installations are assumed to be 100 MW each. Renewable energy from the grid is not used to satisfy the remaining demand for current. The optimizer finds the LCOE when there is a restriction on the size of the renewable energy park and will still have to meet the annual demand for hydrogen. For scenarios 3 and 4, the production is assumed to be done at a place where the weather characteristics are much more suitable to establish a wind/PV park. So in these scenarios, the need for hydrogen pipelines arises to transport the produced hydrogen to the respective industry. The investement costs for these are included in the cost calculations.

Scenario	**Location**	**Renewable Park Size**	**Pipelines**	**End User**
1	Berlin	No Restriction	No	Industries
2	Berlin	100 MW Wind and PV each	No	Industries
3	Berlin	100 MW Wind and PV each	100 km	Industries
4	Berlin	100 MW Wind and PV each	200 km	Industries
5	Berlin	No Restriction	No	Mobility sector
6	Berlin	100 MW Wind and PV each	No	Mobility sector

Table 4: Scenario Matrix for Path 2

Then two more scenarios are simulated for Berlin where the demand is for the mobility sector. The demand curves for mobility sectors are taken as explained in section 6.4. This is then used to run the simulation for Berlin.

5 Simulation Methodology

Simulation is defined as the imitation of the operation of a real-world process or system over time [25]. One of the most important part in a simulation is giving the simulator inputs that represent the real life scenario as close as possible. The other important aspect is choosing the type of simulation. The basic types of simulation are as follows :-

- Static or Dynamic
- Deterministic or Stochastic and
- Discrete or continuous

Static simulation are not based on time whereas dynamic simulation includes the passage of time too [26]. Usually samples are drawn and then a statistical output is derived in a static simulation. With deterministic simulation, the parameter values and initial conditions fully determine the output of the model. On the other hand stochastic models possess some in-built randomness. This means that risk-bearing influences are considered.
In a discrete model, the state variable changes only a finite number of times whereas, in a continuous model, the state variables change infinite number of times but still never abruptly.

MATLAB is used to compute and analyse these kinds of models in a numerical environment. Calculations and visualiasations can be done in MATLAB. It is widely used in fields of engineering and mathematics. MATLAB has other toolboxes/packages that makes its use much easier. StateFlow and Simulink are such packages that allow the usage of graphical tools. Stateflow (developed by MathWorks) is a control logic tool used to model reactive systems via state machines and flow charts within a Simulink model [27]. Simulink provides a graphical programming environment for modelling and simulating dynamical system. All these together eliminates the necessity of text oriented programming.
Also a parallel computing toolbox is used in the simulations here. This allows the usage of all available cores in the server to do the optimization simultaneously.

5.1 Optimization

Optimization is defined as maximizing or minimizing some function relative to some set, often representing a range of choices available in a certain situation. Mathematically it can be represented as shown below.

$$min\, or\, max f(x) \tag{28}$$

where x ϵ Z.

The optimization are made up of three basic elements. They are :-

- Objective function
- variable
- constraints

These are the building block of an optimisation problem. The objective function is either set to be maximised or minimised. In our case, the optimization function will be the LCOE and it will be minimised. The variables are used to achieve the required results from optimization. The constraints are to make sure that the solution sticks to its confined area called the solution space.

5.2 Optimization methods

The type of optimization method to be used greatly affects the accuracy of the results. This is because, sometimes the number of variables are too high and the optimization problem is so complex that a complete enumeration will take a huge amount of time. Part of the skill while dealing with optimization is to apply constraints wisely to reduce the computational time as well as getting as close to complete enumeration as possible. Also a complete enumeration is possible only if all the involved variable are discrete.

There are two types of optimization method. They are deterministic and stochastic methods. The optimization methods that generate and use random variables are stochastic optimization methods. For stochastic problems, the random variables appear in the formulation of the optimization problem itself, which involve random objective functions or random constraints. Random iterates are also included in stochastic optimization methods [28].

With deterministic method, the algorithms localise at an optimum point of their execution, and have only one path for continuing. Deterministic method mainly consists of gradient based optimization algorithms. Gradient methods are used to solve functions of the form shown in equation 5.2 where the gradient of function at a point defines the search direction.

$$\min_{x \in R^n} f(x) \tag{29}$$

5.2.1 Deterministic optimization methods - Gradient based

Gradients are the centre of this optimization method. A delta operator usually is determined:-

$$\Delta f = \left(\frac{\partial y}{\partial x_1}, \dots \frac{\partial y}{\partial x_n} \right) \tag{30}$$

The partial derivatives of the target function according to the variables are specified by the delta operator. An arbitrary solution and step factor is used to generate a new solution vector for the next iteration.

$$x^{(i+1)} = x^{(i)} - \Delta f(x^{(i)}) \tag{31}$$

The method converges with appropriate choice of step size factor and target function. The problem with this method is that there is no guarantee that the optima can be found. This is because in case of small slopes, the optimum is skipped. Also large computational time is required. The step size also adds further complication. If it is too large, the gradient accuracy is poor. If it is too small, the gradient is too large. Like all other methods, specific adaptation of this method to the optimization problem is highly critical to get the right optimum.

5.2.2 Stochastic optimization methods - Evolutionary algorithms

There are many classes of stochastic optimization methods. Popular authors classify it in the following ways [29] :-

- Random search algorithms
- Probabilistic search algorithms
- Metaheuristics
- Partion based stochastic

In the partition based stochastic approach the solution space is divided and the optimum in that space is found. With random search algorithm, minimal information is used for optimization and hence high computing times. With probabilistic search, the algorithm searches in the solution space using an probability distribution. The most popular method is the evolutionary algorithm method.

Evolutionary Algorithms

Evolutionary algorithms use the principle of evolution. The way this works is that a start-up population is created. It uses process inspired by biological evolution. These are reproduction, mutation, recombination and selection. The following steps are followed in an algorithm executed by evolutionary algorithm :-

1. A Start-up population is created.
2. The fitness of the individuals in the start-up population is evaluated.
3. The following steps are repeated until the specified stop criteria
    - Selection of best fit individuals for further population creation.
    - Crossover and mutation is done to breed new offspring.
    - Fitness of new individuals to be evaluated.
    - Replace population with low fit with the ones with higher fit.

Recombination or crossover is the crossing of two individuals and mutation a random change in the genes. The advantage is the this method can be done parallely easily and can save computational time with parallel workers. Although enormous storage capabilities are needed to do this type of computation

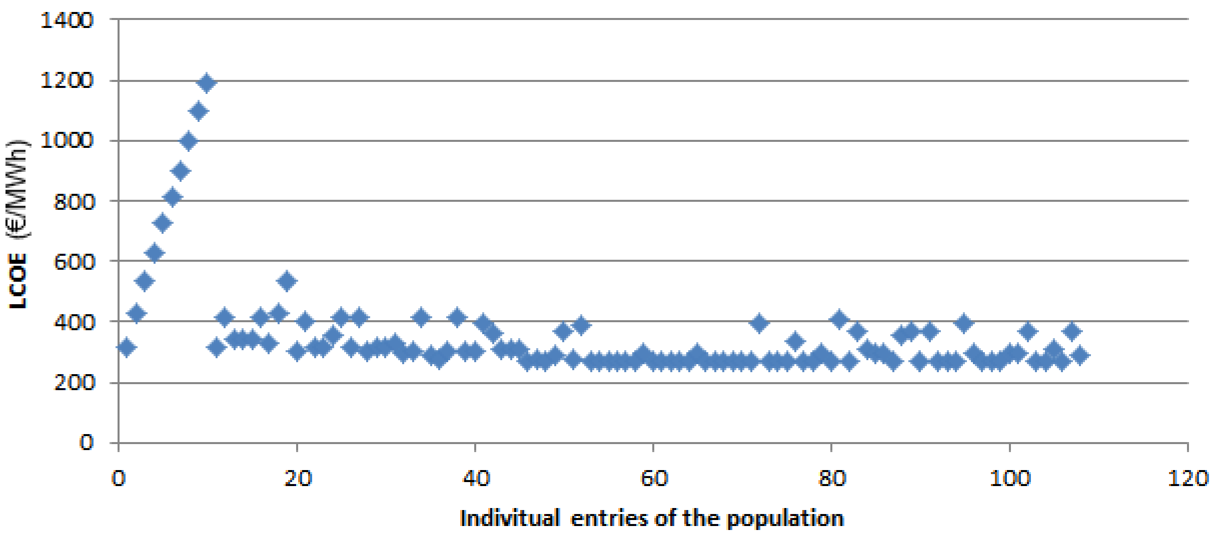


Figure 19: Evlolutionary Algorithm - LCOE

Figure 19 and 20 shows the values used during the entire simulation. In the beginning, the creation of a starting population can be clearly seen by the first 10 points. There are 10 points in almost a straight line here. This is because, for parallel computing, 10 parallel workers are created and 10 sets of starting population are created.

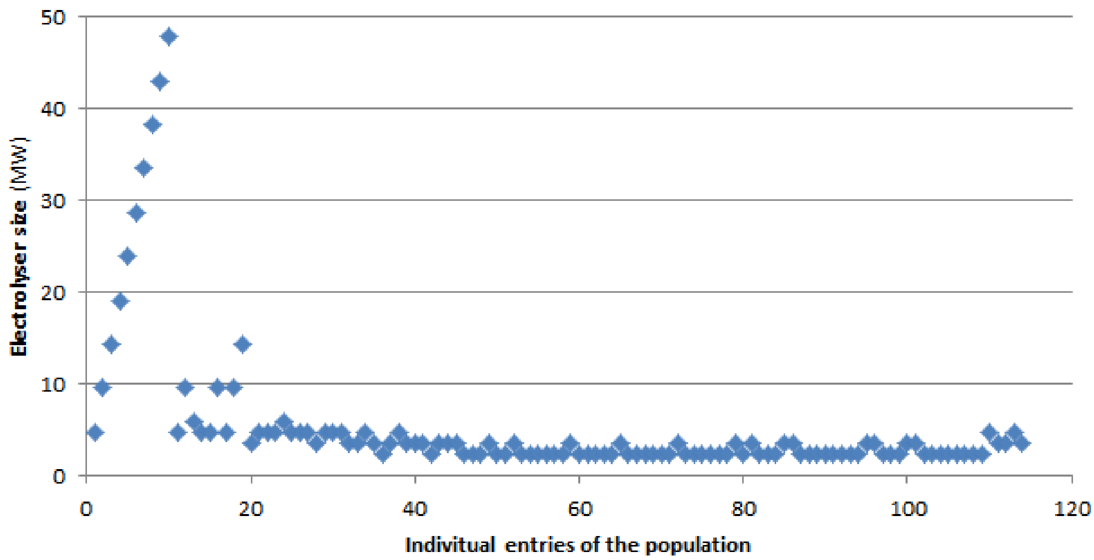


Figure 20: Evlolutionary Algorithm - Electrolyser size

6 Optimization Variables

The optimization is carried out with the optimization tool box in MATLAB. Various inputs have to considered and this section deals with the inputs and other variables that have been considered in the simulation.

6.1 Electricity Market

The electricity markets in Germany works both on exchange and over the counter methods. There are two exchanges, namely, European Energy Exchange (EEX) in Leipzig and European Energy Exchange (EPEX SPOT) in Paris where standardised products are bought and sold in a transparent environment. Over the counter trading happens when the energy producers and consumer have a contract between them.
Trading can done in three different markets. They are forward, day-ahead and intra-day markets. In a forward market, the deliverables can be agreed for periods of upto 6 years. Spot market includes both day-ahead and intra-day markets. Here short term electricity trading happens. The bids for the next day are submitted by the sellers and buyers in the day ahead market. The cut-off time is until 12 midday of the previous day. The more closer to the cut-off time you are when you are placing your bid, the more the chances are to better estimate the feed-in tariff.

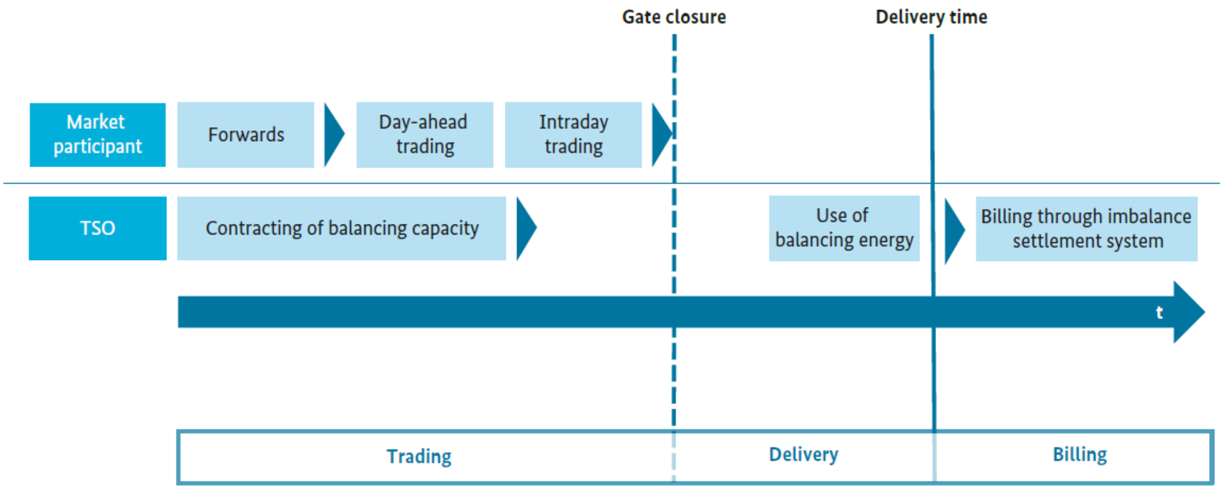


Figure 21: Submarkets in German Electricity market [30]

Intraday market is a much more dynamic environment where the trading is done for a shorter period. This varies from quarter hour blocks to one hour blocks. This is to have a better fit between demand and supply and also to ensure that the surplus and shortfalls are kept to a minimum. This helps in maintaining a cost effective system. The cut-off time in this type of trading is 45 minutes before the time of delivery [30].

The point where the supply and demand meet is the quoted price in the exchange. A merit order is established where the power plant operators are arranged in increasing order of their variable cost. In this system a marginal power plant is identified. Marginal power plant is the plant with the highest variable costs at the exchange price. All the plants operating are remunerated at this cost. Figure 22 shows an example of how a merit order and marginal plants are establied.

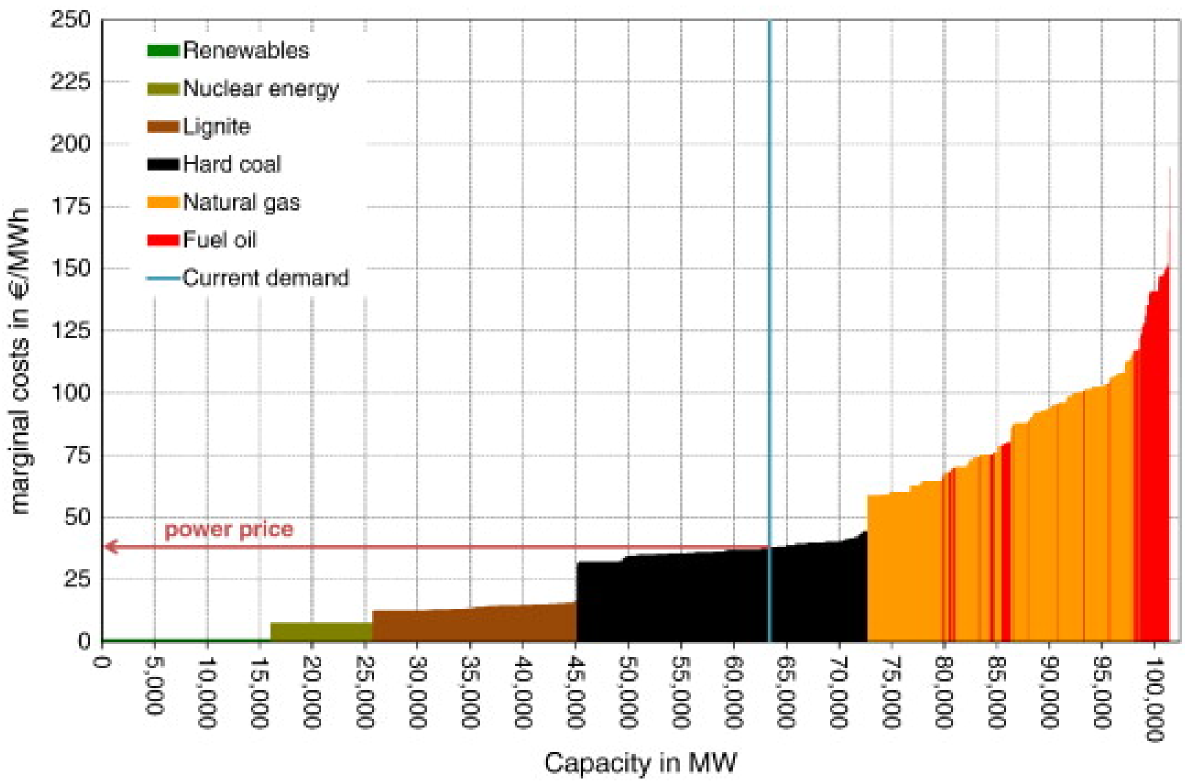


Figure 22: Merit order of common power sources in Germany 2015 [31]

It can be seen from figure 22, that renewables have a marginal cost of almost zero. This indicates that as more renewables are a part of the energy production, the curve moves to the right and the exchange price(power price in the figure) will reduce. Also, this will make the conventional power plants unnecessary to meet the demand. This condition is called as negative residual load. In this scenario, a need arises to switch off installations that produced electricity at a marginal cost higher than the exchange price. Also, the conventional power plants are required to operate under partial load to facilitate better control over power.

The Federal Ministry for Economic Affairs and Energy (BMWi - Bundesministerium für Wirtschaft und Energie) published some ideas for changing the electricity market design in their Green Paper (Ein Strommarkt für die Energiewende - Grünbuch). This became necessary because with increased penetration of renewables, the regulation of power supply became very inefficient as the conventional power plants were rarely used. In the green book, one of the methods recommended was expanding the electricity market using capacity market [30].

In the proposed capacity markets, a secondary market is created additionally. This market deals with only maintaining the capacity and is in turn only remunerated for this. Remuneration of capacity in current market is implicitly done only on forward markets, spot markets and electricity procurement contracts. Based on the studies done in the green paper and as further development to existing German energy market, the Energy market 2.0 is introduced. In order to facilitate the environment described in Energy market 2.0, the Electricity Market Act was adopted in 2016.

6.1.1 Energy Market 2.0

There are three main components in the this proposed new energy market 2.0. They are listed out below [32]:-

- Component 1 : Stronger market mechanisms.
- Component 2 : Flexible and efficient electricity supply.
- Component 3 : Additional security.

Stronger market mechanisms ensures synchronisation between consumption and generation. Also this pushes the companies in the market to maintain enough capacity and utilize them properly. The electricity market will be able to fulfil its synchronisation function which will provide security of supply.
Flexible and efficient electricity supply optimises the supply side. It encourages the suppliers to produce energy in a way that is more environmentally friendly. This encourages more new energy providers (renewables) to step into the scenario and with flexible consumers and a variety of storage options will help these renewable energy provides to actively participate in the balancing of power generation and consumption. This also boosts the competition, which helps in surgically reduce the minimum consumption of conventional power plants. Component 2 will also strengthen the price signals. Also steps to integrate European internal market are being encouraged by Germany. This will help in achieving the goals of energy transition faster and probably cost effective too. With increase in usage of smart meters for houses, more information will be available to facilitate grid operators to be more flexible. Component 3 is the security of supply. This is of the highest order of importance as this ensures that there is no risk of supply shortages. A monitoring process will ensure that there is a possibility to meet demand any time. Also a capacity reserve will be established to safeguard the market. This is different from the capacity market mentioned earlier.

The most important aspect is that this Energy Market 2.0 scenario provides great prospects for new businesses such as battery storage, P2G tp enter. Electrolysers are becoming more and more flexible and this in turn will make the supply side flexible to. All this lead to security of supply which is a very important factor to consider when there are more renewables as a part of production.

6.2 Investment

The accuracy of investment costs taken for different parts of the electrolyser greatly affects the LCOE. Different sources are used to find and decide the investment costs of various parts as accurately as possible.

6.2.1 Electrolyser

The investment cost of electrolyser is based on the size of the electrolyser. Not much data is available in this area. Fraunhofer [3] has data regarding the cost of electrolyser and it's size. This can be seen in table 5.

Investment Cost of Electrolysers - 2017	
Size (in MW)	**Specific Cost (in €/kW)**
0.5	1274
5	1007
100	742
1000	587

Table 5: Investment Cost for electrolyser

Based on the values in table 5, the graph shown in figure 23 is plotted.

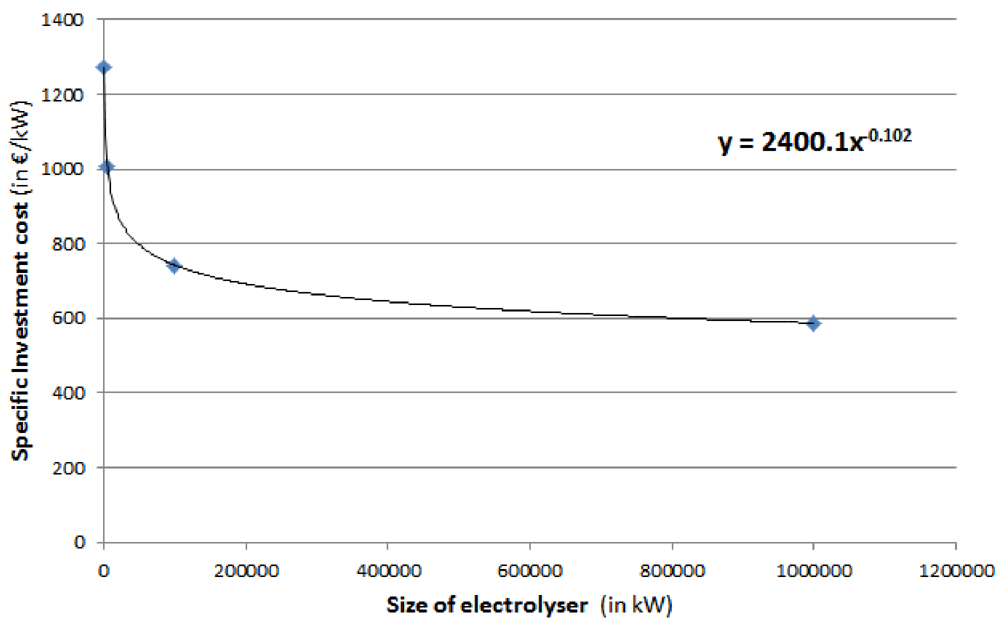


Figure 23: Investment cost calculation for electrolyser

[3]Based on internal communication with project partners

Using the plotted points, a power function trend line is created. Based on this function (seen in figure 23) a lookup table is created in simulink model which will choose the investment cost based on the size of the electrolyser deemed suitable by the optimiser. The same procedure is adopted for the other years, 2030 and 2050 to be specific.

6.2.2 Wind and PV

For wind an PV installation cost, studies have been done on estimating how much a PV or wind installation will cost in future. Also the studies give data on the expected lifetime of the installation, operation and maintenance cost as a factor of investment cost.

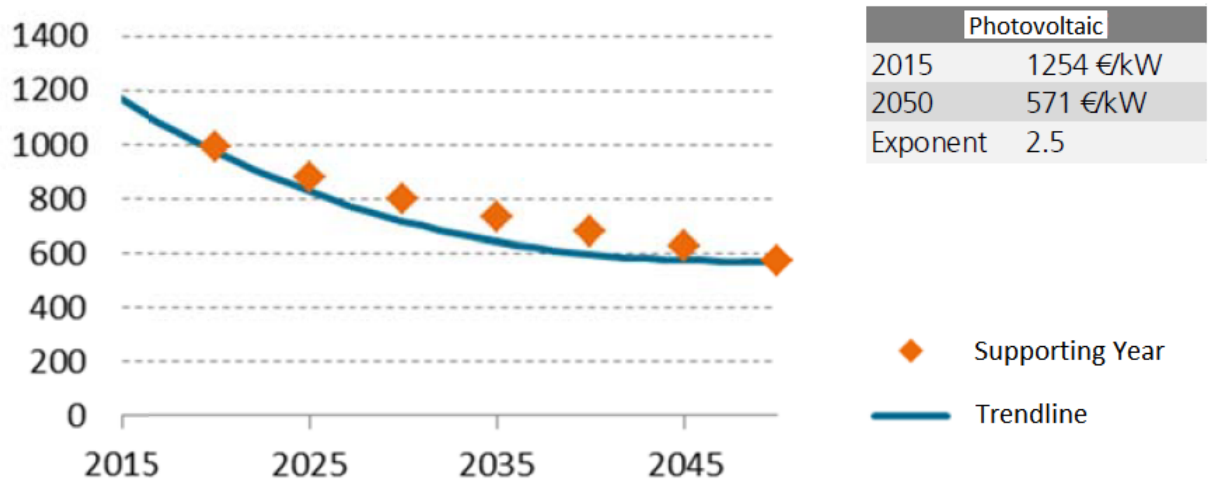


Figure 24: PV investment cost prediction [33]

Figure 24 shows the predicted investment cost for PV in €/kW. Similarly data is available for wind installations.

The operation cost and lifetime of the turbines and PV installations are vary based on the manufacturers, the method of analysis used, and even the location where it is being considered. This can be see in figure 25 [4].

[4] Original table from source modified

Parameter	Germany	Spain	Denmark	UK
Installed capacity [GW] (2015)	45	23	5.1	13.6
% of electricity consumption (2015)	9.7%	17.9%	42.1%	13.3%
O & M costs [cent/kWh] (2013–14)	3.1	2.9	1.7	2.8
Operators	Many/ small	Few/ large	Many/ small	Many/ small-large
Site availability	Limited	Many	Limited	Many

Figure 25: Operation and Maintainance cost for Wind installations in different parts of Europe [34]

Standards have been agreed on which models can be used to estimate the lifetime and other parameters of the installation. Based on this the values for lifetime and operating costs for wind and PV installations are estimated. These are used for the calculations in the optimization.

6.2.3 Storage

Cost and life of the storage are obtained in a method similar to the one followed in section 6.2.1. The investment cost of storage, its lifetime and operational costs are determined by talks with projects partners/suppliers [5].

6.3 Economic Feasibility

There are many established methods to analyse the economic viability of the project. Investment assessments are done to compare projects. These accounting methods take into account all the expenditure and incomes that will occur over the lifetime of the project. When comparing different methods of energy production, comparing the energy production costs is more suitable.

The capital value of an investment can be used ot compare the profitability or the economic feasibility of the project. Capital value is the difference between all the revenues and all the expenditure based on a reference date [35]. Equation 32 shows how it is calculated.

$$K_0 = -I_0 + \sum_{t=1}^{n} \frac{E_t - A_t}{(1+i)^t} \tag{32}$$

Where,
K_0 is the capital value at reference time in €,
I_0 is the investment expenditures in €,
E_t is the revenue in year t in €,
A_t is the expenditure in the year t in €,
i is the calculating interest rate,

[5]Based on internal data from Fraunhofer-ISE

t is the respective year of operation.

Usually the date of commissioning an installation is suitable as t. If the capital value is positive, then the project is economically viable. If the capital value is negative, then the project is not economically viable.
Projects usually involved in production of energy is compared using their LCOEs. LCOE stands for Levelised Cost of Energy. It is nothing but the cost to produce one unit of energy. It is more suitable to use this method as most of the energy projects have their LCOEs calculated and calculating the same for hydrogen production in P2G pathways will give us a good platform to compare. The LCOE is calculated using the equation 33.

$$LCOE = \frac{I_0 + \sum_{t=1}^{n} \frac{A_t}{(1+i)^t}}{\sum_{t=1}^{n} \frac{W_t}{(1+i)^t}} \tag{33}$$

Where,
LCOE is the Levelised Cost of Energy in €/kWh
I_0 is the investment expenditures in €,
A_t is the expenditure in the year t in €,
W_t Annual Energy Production in kWh,
i is the calculating interest rate,
t is the respective year of operation.

In is rational to assume that the generation and expenditures incurred by the plant annually would fairly be constant throughout its lifetime. So the annuity method can be used to calculate the LCOE. In this method, the expenditure and generations are converted to an equivalent annual cost using the annuity factor. This factor is calculated using the equation 34.

$$ANF = \frac{1}{\sum_{t=1}^{n} \frac{1}{(1+i)^t}} \tag{34}$$

Where,
ANF is the Annuity factor,
t is the respective year of operation.
n is the lifetime.

Equation 34 on further simplification gives us the following:-

$$ANF = \frac{(1+i)^n \cdot i}{(1+i)^n - 1} \tag{35}$$

This annuity factor can be multiplied with the investment costs and this distributes the investments equally. From equation 35 and 33, LCOE can be calculated as follows:-

$$LCOE = \frac{ANF \cdot I_0 + A_t}{Wt} \tag{36}$$

When comparing different technologies using LCOE, the system with the lowest LCOE is the most economical. Also the LCOE gives information on what range the selling price of the produced hydrogen might be.
With respect to the simulation being done in the scope of this thesis, other parameters such as the operational expenditure (OPEX), residual value (Residual) and Reinvestment cost (Reinvest) are to be included. The equation 37 shows the formula to calculate the LCOE that is used in the simulation.

$$LCOE = \frac{CAPEX + \sum_{t=1}^{n} \frac{OPEX_t}{(1+i)^t} + \frac{Reinvest}{(1+i)^t} - \frac{Residual}{(1+i)^t}}{\sum_{t=1}^{n} \frac{W_{out}}{(1+i)^t}} \tag{37}$$

As done earlier, the reinvest and residual must be converted into constant payment to compute the LCOE by annuity method. For this purpose a residual value distribution factor (RVDF) is created as shown below:-

$$RVDF = \frac{i}{(1+i)^n - 1} \tag{38}$$

The one time payment of reinvest or the residual can be converted to a continuous payment series by multiplying it with RVDF.

$$\sum_{t=1}^{n} \frac{Reinvest \cdot RVDF}{(1+i)^n} \tag{39}$$

From equation 34, transformation can be applied in the equation 39 as shown below:-

$$\sum_{t=1}^{n} \frac{RVDF}{(1+i)^n} = \frac{RVDF}{ANF} = \frac{i}{(1+i)^n - 1} \cdot \frac{(1+i)^n - 1}{(1+i)^n \cdot i} = \frac{1}{(1+i)^n} \tag{40}$$

Therefore, equation 37 becomes :-

$$LCOE = \frac{CAPEX + \sum_{t=1}^{n} \frac{OPEX_t}{(1+i)^t} + \frac{Reinvest \cdot RVDF_1}{(1+i)^t} - \frac{Residual \cdot RVDF_2}{(1+i)^t}}{\sum_{t=1}^{n} \frac{W_{out}}{(1+i)^t}} \quad (41)$$

RVDF are different for different components like reservoir, stacks, cavern, etc. as the payments are done in different years. The residual values of all the invested entities are taken into account by their respective RVDFs based on their expected lifetime.
Also, the system is desinged to work in such a way that the total amount of hydrogen produced is equal to the total hydrogen demand. This is a ratio of the produced hydrogen per year to the total annual hydrogen demand . If the ratio is less than one, this means there was lesses use of electricity and this was also included into the calculation of the LCOE.
There is a difference in storage loading at the beginning and end of the year, if the hydrogen produced is less. This is included as an annual cost in the next year. Including all that have been mentioned, we get the final LCOE formula (equation 42[6]) as shown below:-

$$\begin{aligned} LCOE = & \frac{ANF \cdot CAPEX + OPEX + ANF \cdot RSV_{n0} \cdot LCOE \cdot \Delta RSV_n \cdot LCOE}{W_{Used}} \\ & + \frac{Reinvest_{stack} \cdot RVDF_1 - RSV_{n0} \cdot LCOE \cdot RVDF_2}{W_{Used}} \end{aligned} \quad (42)$$

Where,
RSV$_{n}o$ is the initial amount of hydrogen in the storage tank and
ΔRSV$_n$ is the difference between initial amount of hydrogen in the storage tank and the amount of hydrogen at the end of the year after simulation.

[6] equation has been split due to lack of space

6.4 Gas Demand

6.4.1 Path 1

The size of the filling station determines the gas requirements. The size is determined by the project. It is decided that it will be a large size refilling station. An average of 700 kg of hydrogen per day and a maximum of 1000 kg per day is the demand for the decided size of the refuelling station [36]. Now a demand profile for this hydrogen is necessary. As reference, the demand profiles of gasoline and diesel was taken. This is under the assumption that hydrogen replenishment need will be the same as that of gasoline and diesel. Monthly consumption of of gasoline and diesel was detemined based on the data available from the Mineral Oil assosication [37].

6.4.2 Path 2

The gas demand for the second path is primarily for an industry. Based on projects such as Chemcoast and HYPOS, a cavern size of 500,000 m^3 and a electrolyser of size 1GW seemed to be a good estimation [38]. Assuming full load hour of 2000 hours, we get a demand of 450 x 10^6 Nm^3 annually.

6.5 Electricity Price

Day-ahead electricity price is dealt with on a hourly basis. The electricity prices are taken from the European Power Exchange(EEX) [39].
There are also a variety of legal framework that affects the price of electricity or in this case, some taxes have to be paid based on the purpose for which the electricity taken is being used.

Duty	Additional Cost for electricity	Source
EEG - Tax	6.24 ct/kWh	EEG
StromNEV - Tax	Until 1000 MWh : 0.187 ct/kWh After 1000 MWh : 0.025 ct/kWh	StromNEV
Offshore - duty	Until 1000 MWh : 0.25 ct/kWh After 1000 MWh : 0.025 ct/kWh	EnGW
KWKG - duty	Until 100 MWh : 0.178 ct/kWh After 100 MWh : 0.025 ct/kWh	KWKG
Concession duty	After 100 MWh : 0.11 ct/kWh	KAV

Table 6: Taxes/duties on electricity used

Table 6 shows the taxes / duties on the electricity being used [7]. The Erneuerbaren-Energien-Gesetz (EEG) and Energiewirtschaftsgesetz (EnGW) deal with the generation, feed-in and utilization of the gas produced [40],[41].

[7] The taxes mentioned here are for the year 2014

KWKG stands for Kraft-Wärme-Kopplungs-Gesetzthe (Cogeneration law [8]). The purpose of this law as defined by the federal government (in 2009) is as follows:-
"The purpose of the Act is to contribute 25% to the increase in electricity generation from cogeneration in the Federal Republic of Germany by temporary protection, the promotion of the modernization and the new construction of cogeneration plants (cogeneration plants) the support of the market launch of the fuel cell, as well as the promotion of the new and expanded heat exchangers to which heat from cogeneration plants is fed in the interests of energy saving, environmental protection and the achievement of the climate protection targets of the federal government [9]."
In EEG, the gas from P2G is considerred as storage gas only "if the gas is solely produced for the temporary storage of electricity from renewable energy sources". Also For P2G systems with coupling of the mobility, the tax has to be paid. The offshore duty has to be paid as it ensures non-faulty liability for disruptions in power from offshore wind plants.
The NEV - Tax are for individual grid charges. The operators of transmission networks are obliged to reimburse lost revenues resulting from individual network charges to downstream operators of electricity distribution networks. The transmission system operators have to compensate these payments as well as their own lost revenues. The lost proceeds are allocated to all final consumers (LV) proportionally to the network charges (StromNEV - Tax).

6.5.1 Others

Wind Share(Windanteil) and **Green Share**(Grünanteil) are also inputs to the simulation. These are the parameters that give the share of renwables in the produced current. Wind Share gives the share of power generated from wind energy in the grid and for the green share, wind turbines, hydro power operators and photovoltaic plant operators are combined together.

Ambient temperature and **soil temperature** data from Hamburg-Neuwiedenthal is also an input.The reference year for this data is 2014. The data is sampled for intervals of 5 minutes. Also, soil temperatures at a depth of 0.5 m were taken at the same location. These values are obtained from the Fraunhofer ISE internal data collection. Also for the second pathway, the weather data, that is, the ambient air temperature for the locations considered is collected from the online data base from the Deutscher Wetterdienst [42].

6.6 Hydrogen storage

Hydrogen storage is a very important part of this simulation. Onsite service stations are used to store hydrogen underground. This is taken into consideration in both the detailed and simple simulations. The maximum pressure of the electrolyser is taken at the maximum storage pressure which is 30 bar. The schematics of the electrolyte model is shown in figure 26

[8] Roughly translated from German
[9] Translated from German

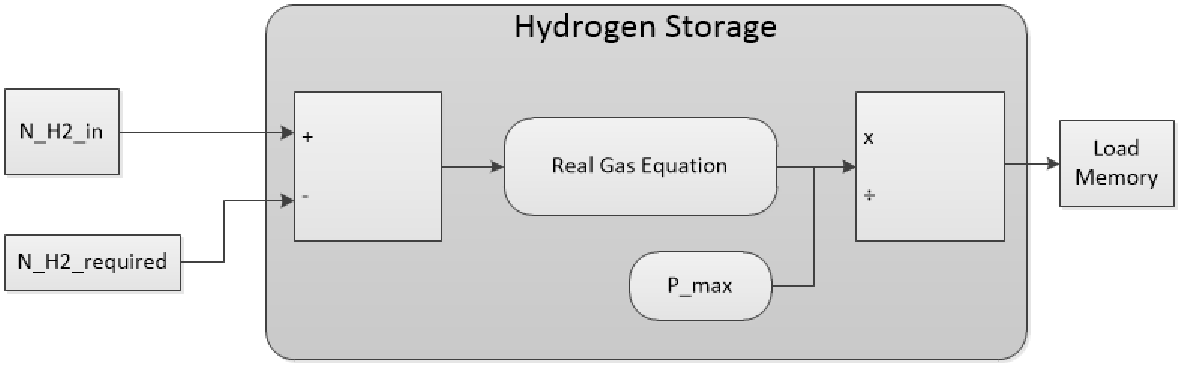


Figure 26: Schematic drawing of hydrogen Storage[18]

In the simplified model, the difference between the amount of hydrogen produced and the amount of hydrogen required is integrated and this gives us a load function(load memory in figure 26). This is then expressed as a function of storage pressure in the storage tank. This is shown in equation 43.

$$\chi_{RSV} = \frac{P}{P_{max}} \tag{43}$$

Where,
χ_{RSV} is the load memory,
P is the storage pressure in Pa,
P_{max} is the max. storage pressure in Pa.
In the detailed model, more inputs are taken into consideration. These include thermal effects such as heat transfer between the soil and gas, pressure as a function of storage temperature. As mentioned in section 4.5, the Soave-Redlich-Kwong equation is used to calculate the pressure.

Parameters	
Min. Storage Pressure	4 bar
Diameter	1.4 m
Tube length	100 m
Wall thickness	0.05 m

Table 7: Parameters for Storage tank [43]

The parametersof the storage tank can be seen in table 7.

In path 2, for the storge of hydrogen, a cavern is used to store the hydrogen produced. Parameters such as volume of the cavern, minimum and maximum storage pressure, ambient temperature, etc. are used to model the cavern.
One of the project partners, DBI Gas und Umwelttechnik Gmbh are dealing with the cavern

modelling and they have provided the model that has been used in the simulation. The parameters can be seen in table 8.

Parameters	
Min. Storage Pressure	60 bar
Max. Storage Pressure	190 bar
Ambient Temperature	40 °C
Cavern Volume	500,000 Nm^3
Max. Input /output Rates	13.5 t/h

Table 8: Parameters for Cavern Storgage [44]

6.7 Electrolyser

The basic parameters of the electrolyser is shown in table 9.

Parameters	
Rated AC Power	1.25 MW
Rated Production	225 $Nm^3 H_2/h$
Lifetime of stack	30000 hours
Operating Pressure	32 bar
Operating Temperature	60 ° C

Table 9: Parameters for electrolyser [19]

The knowledge on electrolysers of 1 MW scale is limited and the values displayed in the table 9 are based on assumptions and approximations from studies [45]. The parameters are that of a Siemens SILYZER 200 stack. There are differences in the model for electrolyser in simple and detailed models, which are dealt with in detail.

6.7.1 Simple Model

The schematic of a simplified electrolyser model is shown in figure 27 [10].

[10] Figures from source [18] have been translated from German for better understanding

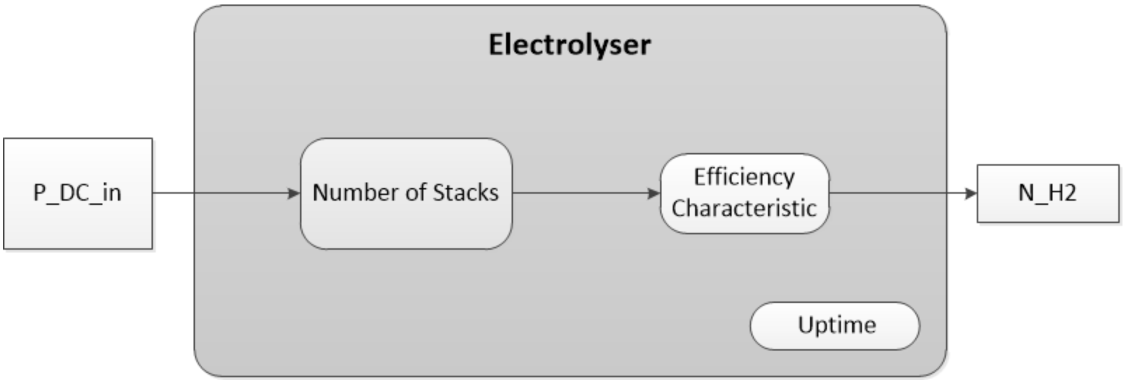


Figure 27: Simple electrolyser model [18]

The input to the model is the DC power. The standard efficieny curve is used to find the efficiency of the electrolyser based on the input power. This is done with the help of a lookup table in simulink, which has the values of efficiency at different levels of DC power and also interpolates the values in between. The string are operated in series, which means a new string is not used until the previous one reaches rated power.

6.7.2 Detailed Model

In the detail model, additional parameters like heat losses, changing efficiencies with changing working temperatures, pumps to ensure water circulation, etc. are considered. Also switch-on times which is due to the time necessary for working pressure to build up are also factored. The basic schematic can be seen in figure 28.

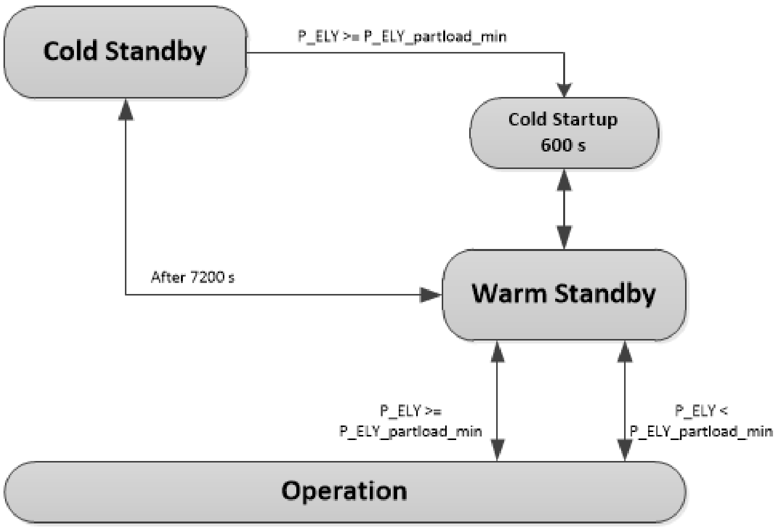


Figure 28: Detail electrolyser model [18]

In the 'operation' state, the electrolyser works under normal temperature and pressure. The output of the electrolyser can be directly quantified by the information specified the manufacturer under these conditions.
Cold start-up is the phase where the electrolyser prepares for start up. The pressure is build

up to the operating range. After the operating temperature and pressure is reached, the electrolyser will go to warm standby mode.

6.8 Modes of Operation (Path 1)

The operation of a power to gas plant can be done based on various deployment strategy. For example, the system can be operated continuously and is switched off only when the maximum allowed storage limit is reached. This might not be the most economical operational strategy as the plant might run when the electricity is very expensive. A price signal strategy can be adopted for the operation of plant as it considers the price of the electricity used to run the electrolyser among all the other variables.

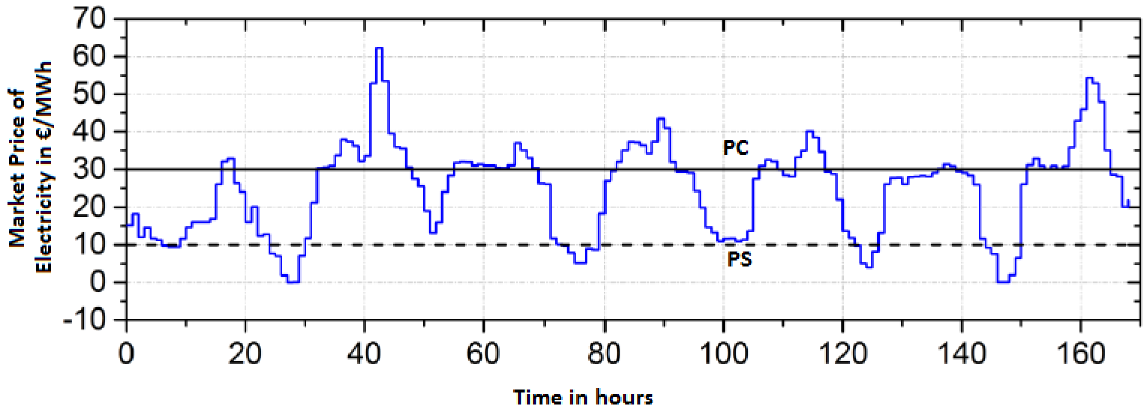


Figure 29: Price Signal(PS) and Price Cap(PC) shown in a weekly Market Electricity Cost

In this strategy, when the cost of electricity is lower than a particular fixed value,the plant is operated at nominal load. This value is the Price Signal(PS) and this mode of operation is called volllast. In order to provide a more organised operation, another control variable called the Price Cap(PC) is introduced. This PC prevents the system from running at times when the price of the the electricity is very high. Figure 29 shows the PS and PC. If the cost of electricity is in between PS and PC, then the plant will operate following the demand This mode of operation is called as teillast. If the electricity price is higher than the PC, then the system will go not be operated. At times when the price of electricity is higher than PC but the storage level is lower than its fixed min value, then the plant will follow the demand. This operation mode is called as stillstand. Figure 30 gives a modest illustration of the modes of operation.

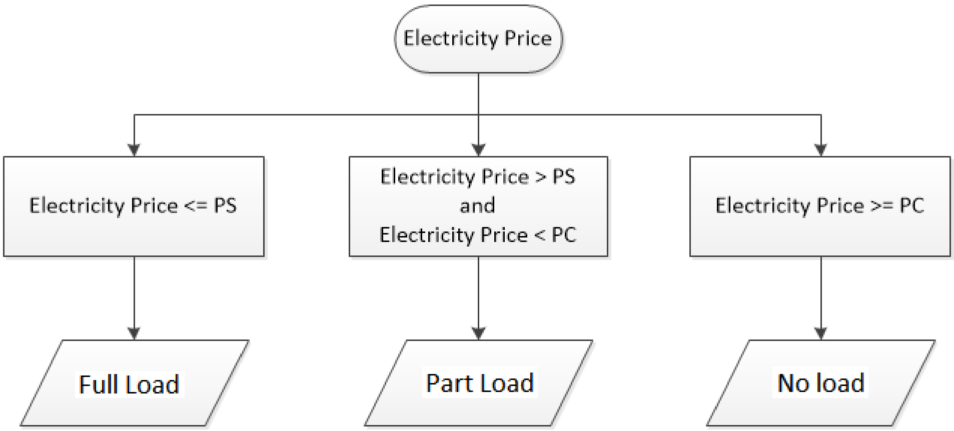


Figure 30: Operation Strategy [18]

The operation strategy determines the power input to the electrolyser. As seen earlier, there are three modes of operation. The current storage capacity, determines the target capacity however, it is highly important to avoid pressure overloading in each and every modes of operation. So based on the load memory defined in the section 6.6, a maximum and minimum memory loads are defined. Based on the experience with the hydrogen storage at Fraunhofer ISE, the minimum and maximum memory loads are taken 2 bar more and 2 bar lesser than the derived values. Figure 31 shows the schematic of operation mode "Full Load".

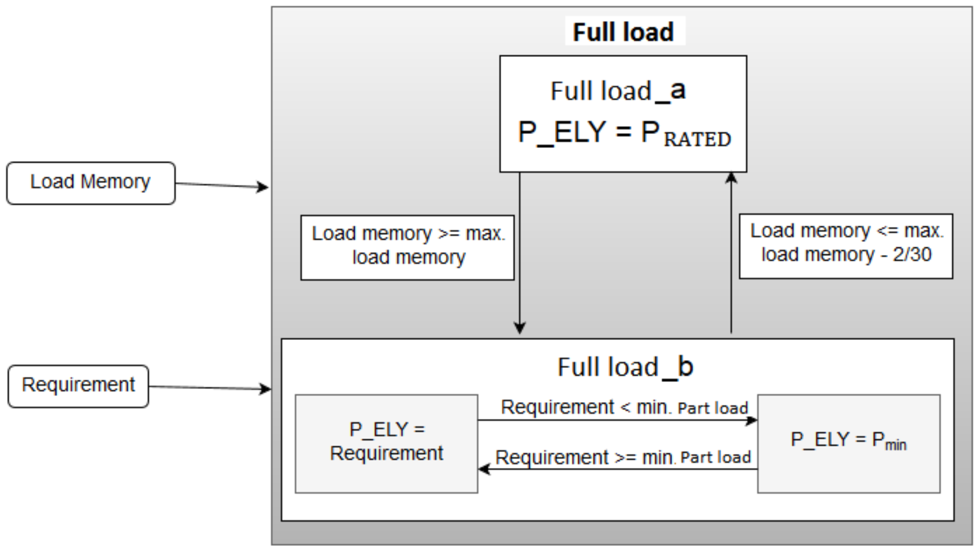


Figure 31: Full load [18]

In the operation mode "Full load (Volllast)", there are further two more states, a and b. The state Full Load_a is when the storage is not full. Here the electrolyser input is set to its rated power. the Full Load_b is when the storage is greater or equal to maximum storage load. This is to ensure that the electrolyser doesn't function when the storage levels are high. Also to avoid constant switching on and off the electrolyser, a hysteresis loop is created. An additional 1/15

P_{max} is added for this purpose. The hysteresis is show in the figure 32 [11].

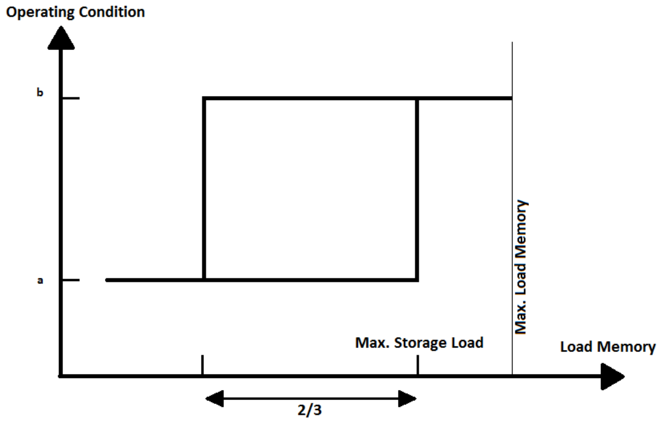


Figure 32: Hysterisis [18]

In the operation mode ”Part load (Teillast)”, It is similar to ”Full load” operation. The necessary power for operation is determined based on the storage levels. Two modes a and b also exists here. A hysteresis loop similar to the one for Volllast operation is implemented between the Part load_ a and Part load_ b modes. The logic of operation mode ”Part load” is shown in figure 33.

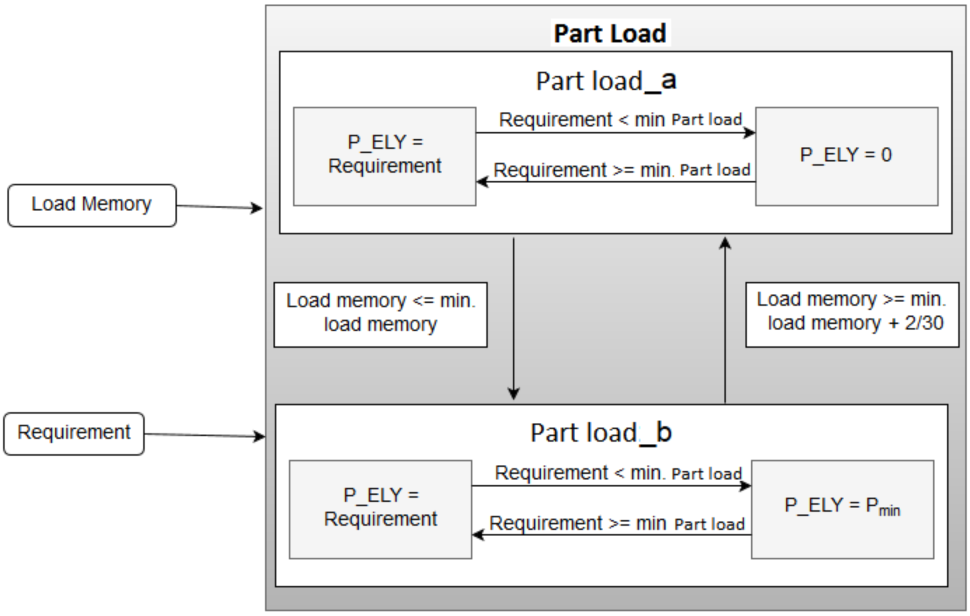


Figure 33: Part Load [18]

[11] Figures from source [18] have been translated from German for better understanding

The operation logic for No load (stillstand) operation is shown in figure 34. Here the electricity price is greater than the defined PC. When the storage load reaches the minimum storage level, the electrolyses is set to produce hydrogen based on the demand. If the storage level is greater than the min storage level, the electrolyser power is set to zero(stillstand_ a in figure 34).

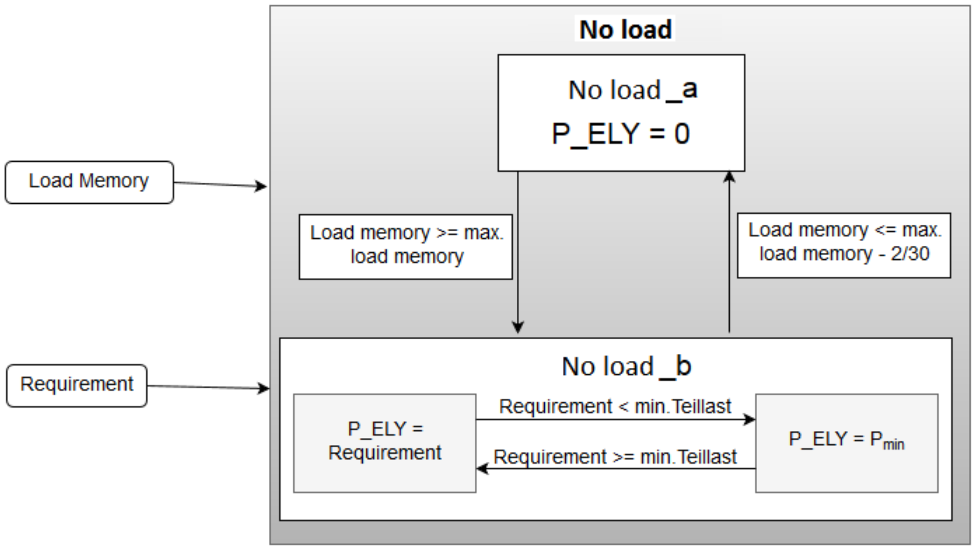


Figure 34: No load [18]

6.9 Modes of Operation (Path 2)

The demand side for the pathway being considered here is industries for the major part. So the demand is fairly constant and not dynamic enough for using the method of Price Signals and Price Caps. The main objective here is that as long as the cavern maximum storage capacity is not reached, useful power from wind and pv will be used to produce hydrogen. The modes of operation are the same as in the previous pathway, namely **Full load**, **Part load** and **No load**. The criteria that chooses one of the earlier mentioned operating modes is different.

Since the scenario here is based on the renewable energy park, the power from it is used as the criteria for control. Installed capacity of the electrolyser system (x_ELY) and minimum DC load defined for the electrolyser system (ELY_ P_ min) are used as the variables for control. The mode of operation can be seen in figure 35.

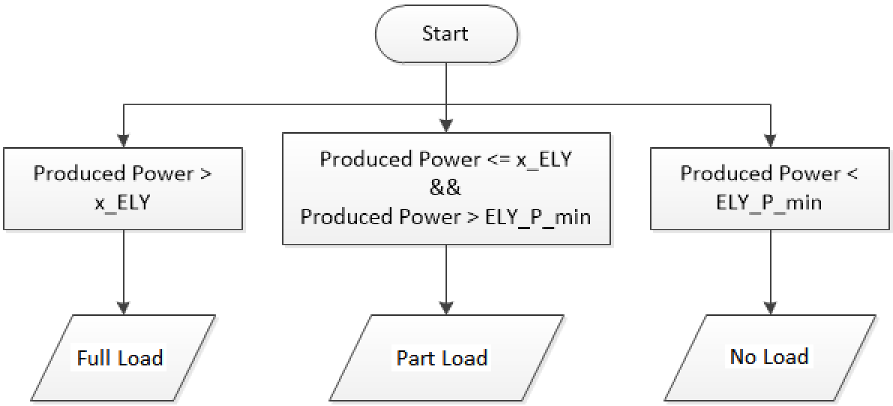


Figure 35: Pathway 2 Operation Strategy

As shown, when the produced power is more than x_ELY the operation mode Full Load is chosen. When the produced power is less than x_ELY but more than than ELY_P_min, the operation mode Part Load is chosen. The operation mode stillstand is chosen when the produced power is less than ELY_P_min. Similar to the mode of operation in the pathway 1, each operation modes have sub modes. For the operating mode No load, there are no sub modes. The electrolyser input is set to zero.

With the operating mode, **Full Load**, care has to be taken that the maximum storage limit. Hence two sub modes Full load_a and Full load_b are created. The mode full load_a, the accumulator load is lower than the maximum accumulator loading. Here the electrolyser power is set to the rated power (P_rated). Figure 36 shows the schematic of the logic for the full load mode.

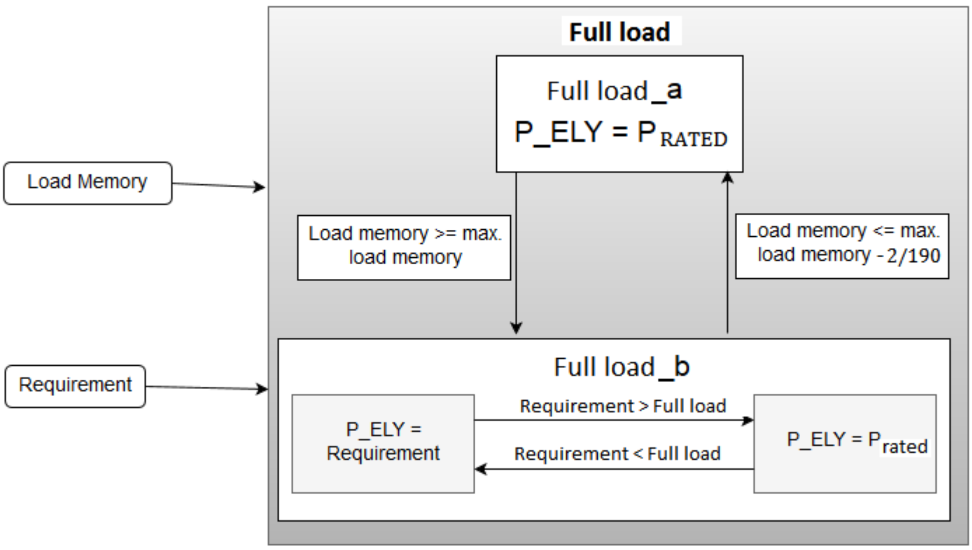


Figure 36: Full load - Path 2 [18]

In the mode full load_b two sub modes are present. Here the requirement is compared with the full load and if the requirement is greater, then the electrolyser input is set to rated power. Else, the electrolyser power is set based on the requirement. The Full load_b mode is chosen only when the accumulator load is greater than the maximum accumulator loading.

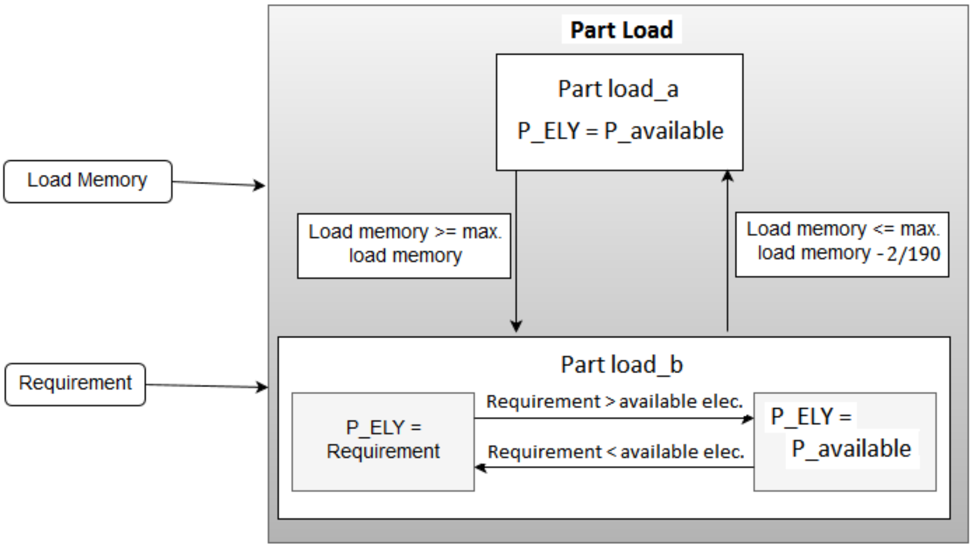


Figure 37: Part load - Path 2 [18]

Figure 37[12] shows the schematic of operation mode part load. The sub modes Part load_a sets the input to the electrolyer as the available power from the renewables. Based on the accumulator loading, the operation mode Part load_b is selected. In this further two modes exists which are chosen by comparing the requirement of the electrolyser and the available power. If the power required by the electrolyser (calculated based on the demand for hydrogen) is more than the available power, then the electrolyser input is set to available power. Else the power is set to value calculated based on the requirement. This ensures that the the maximum accumulator loading is not crossed.

[12]Figures from source [18] have been translated from German for better understanding

7 Simulation Results

Simulations were done for various scenarios depicted in tables 3 and 4. The simulations times are different for the simple and detailed models and only few of the scenarios for both pathways were run in the detailed simulations. The following Key Performance Indicators (KPIs) were identified as a common ground to compare the results of the simulation for various scenarios.

7.1 Key Performance Indicators

One of the primary grounds for comparision of the results from various scenarios are the LCOE. This gives us an exact picture of how much per the end user must pay for a unit of energy produced in the pathway.
For the first pathway, the Price Signal (PS) and Price Cap (PC) are chosen as one of the KPIs. This directly reflects on the operation strategy of the system in the scenario. For example, if the PS and PC are the same value, then this indicates that the system basically follows an on and off opeation. The size of the reservoir (speicher) in m^3 is also provides us with some useful information.

Then the full load hours (VLS) of the system is another KPI as this gives us information on the loading of the electrolyser. Equation 44 shows how the VLS is calculated.

$$Full\,load\,hours(VLS) = \frac{Annual\,amount\,of\,hydrogen}{Installed\,electrolyser\,size} \tag{44}$$

The number of complete cycles that the reservoir/storage is used for also gives us an insight into how the system has been working. More the storage cycle, more the reservoir is being used to meet the demand.

$$Full\,load\,storage\,cycles = \frac{Hydrogen\,fed\,to\,the\,storgage}{maximum\,storable\,amount\,of\,hydrogen} \tag{45}$$

Below you can see the mathematical expression for the same:-

$$Full\,load\,storage\,cycles = \frac{\int_0^t \Delta n \cdot t}{(\rho_{P_{max}} - \rho_{P_{min}})\,V_{storage}} \tag{46}$$

where, $\rho_{p_{max}}$ is the density of hydrogen at maximum pressure,
$\rho_{p_{min}}$ is the density of hydrogen at minimum pressure and,
$V_{storage}$ is the volume of the storage tanks

The Windshare (windanteil) and Greenshare(Grunanteil) are the other parameters that tell us how much of the produced hydrogen is from electricity produced by wind energy and renewable energy respectively. This basically gives us the information on what type of current is used. Equations 47 and 48 show us how the same is calculated.

$$Windshare = \frac{Drawn\,Windpower}{Total\,amount\,of\,electricity\,purchased} \tag{47}$$

$$Greenshare = \frac{Drawn\,greenpower}{Total\,amount\,of\,electricity\,purchased} \tag{48}$$

The greenshare includes electricity from all renewable sources such as wind turbines, PV plants, hydropower, etc. The windshare considers only the electricity from wind power.

For the path two, where the power is supplied only from the wind and PV plants, it is interesting to know the LCOE of these components (wind and PV). This gives us an insight into the current production costs. For this the respective LCOEs are calculated. Equations 49 and 50 shows how the calculation is done.

$$W\_LCOE = \frac{CAPEX_{wind} \cdot ANF_{wind} + OPEX_{wind}}{Drawn\,Windpower} \tag{49}$$

$$PV\_LCOE = \frac{CAPEX_{PV} \cdot ANF_{PV} + OPEX_{PV}}{Drawn\,PV\,power} \tag{50}$$

Also to analyse the path 2 information on the electricity being used is useful. For this purpose two other KPIs are used. The Wind$_{usage}$ gives data on how much of wind energy is used for the production of hydrogen. It is calculated as shown in equation 51.

$$Wind_{usage} = \frac{Consumed\,Wind\,electric\,Energy}{Total\,Possible\,wind\,electric\,Energy} \tag{51}$$

Similarly, the PV$_{usage}$ usage gives us information on how much of the usage is from PV. The equation is shown below:-

$$PV_{usage} = \frac{Consumed\,PV\,electric\,Energy}{Total\,Possible\,PV\,electric\,Energy} \tag{52}$$

7.2 Path 1 Results

The results from the simulation are obtained for all the reference years based on the concepts mentioned in the previous sections. The KPIs are calculated using the formulae mentioned in section 7.1.

7.2.1 Year 2014

The results for the year 2014 in a full tax scenario is shown in the figure 38.

Scenario	Operation	Comb. Price	50% RE - var Storage
	Taxes	full	full
	Year	2014	2014
LCOE	€/MWh	268.49	291.3109
	€/Kg	8.941	9.70065297
PS (€)		55	31
PC (€)		63	38
Storage (m³)		82	74
Green Share		0.22	0.22
Wind Share		0.11	0.11
Full load hours (ELY)		6334.9893	6334.9892
Efficiency (%)		0.53227574	0.54103701
Storage Cycles		190.14996	276.63467

Figure 38: Result - 2014 Full tax

The Comb. Price operation more is the type of operation that has been explained in section 6.8. The 50% RE-var Storage mode is an operation strategy where the system is run when there is more than 50% renewables. Also there is no boundary condition enforced on the size of the storage and the system is allowed to optimise on this too.

It can be seen that that LCOE increases from 8.94€/kg to 9.7€/kg. The price signal (PS) and price cap (PC) are €55 and €63 respectively. In the variable storage case, the PS and PC are 31 and 38 respectively. It is interesting to note that the storage size has been reduced from 82 m^3 to 74 m^3. This reduction in storage size is justified by increased storage usage cycles (VLSpeicherzyklen) of the storage.

Scenario	Operation	Comb. Price	50% RE - Var. Storage
	Taxes	Reduced	Reduced
	Year	2014	2014
LCOE	€/MWh	159.94	160.53386
	€/Kg	5.326	5.34577754
PS (€)		43	70
PC (€)		63	70
Storage (m^3)		82	70
Green Share		0.22	0.22
Wind Share		0.11	0.11
Full load hours (ELY)		6334.9893	6334.9892
Efficiency (%)		0.53258098	0.53235562
Storage Cycles		188.56644	208.81359

Figure 39: Result - 2014 Reduced tax

Figure 39 shows the results for the year 2014 where the taxes are reduced after a certain consumption. There is only marginal difference in the LCOE between the two strategies. Again the storage size has been reduced from 82 m^3 but to 70 m^3. The PS and PC in the comb.price operation strategy is 43 €and 63 €respectively. In the Var. Storage strategy, the PS and PC can be seen to be the same (70 €). This means that in this scenario, the electrolyser basically operates as on and off. The decreased storage size is compensated by increased storage usage cycles. Comparing these results with the full tax scenario for the same year (figure 38), it can be seen that the effect of electricity price has significant impact on the LCOE. It can be seen that it has dropped from 8.94 €/kg to 5.34 €/kg.

Scenario	Operation	Comb. Price	50% RE - var Storage
	Taxes	Free	Free
	Year	2014	2014
LCOE	€/MWh	151.87	175.58995
	€/Kg	5.057	5.84714534
PS (€)		70	32
PC (€)		70	34
Storage (m^3)		82	92
Green Share		0.22	0.22
Wind Share		0.11	0.11
Full load hours (ELY)		6334.9893	6334.9893
Efficiency (%)		0.53234681	0.53925101
Storage Cycles		178.21373	302.02994

Figure 40: Result - 2014 tax Free

Now figure 40 shows the results for a tax free scenario. It can be seen that the LCOEs of both comb. Price and 50% var. Storage operation strategies are in similar range of that of reduced tax case. This is because the EEG charges are reduced from 62.4 €/MWh to 1 €/MWh after a consumption of 1 GWh. Keeping the consumption of a P2G plant of this scale, the consumption of 1 GWh is easily reached. It is interesting to note that the comb. price operating mode works in just on-off mode (PS and PC are equal). The var storage operating mode works with a PS of 32 €and a PC of 34 €. Here the storage size recommended is 92 m^3. This can be because of the low PS and PC. Also this is why the number of storage cycles are more than the comb. price operation mode.

7.2.2 Year 2030

In this part the results for the year 2030 are shown and discussed. There are a few minor changes in the input given to the optimization tool box. The predicted wind and green share for the years 2030 is used as input whereas in the previous section for the same, the values in the year 2014 are used.

Scenario	Operation	Comb. Price	75% RE - Var. Storage
	Taxes	full	full
	Year	2030	2030
LCOE	€/MWh	248.83	265.64979
	€/Kg	8.286	8.84613801
PS (€)		36	31
PC (€)		67	38
Storage (m^3)		82	74
Green Share		0.64323205	0.63
Wind Share		0.35700945	0.35700945
Full load hours (ELY)		6334.9893	6334.9893
Efficiency (%)		0.53316315	0.54103701
Storage Cycles		178.22771	276.63467

Figure 41: Result - 2030 Full tax

The figure 41 shows the results for the year 2030 in the full tax scenario. It can be observed that the LCOE is 8 .28 €/kg for the comb. price operation mode. The PS and PC are 36 €and 67 €respectively. Whereas for the var. storage operation mode, there is a small increase in the LCOE and the PS and PC at 31 €and 38 €respectively are lower. Also the storage is deemed to be optimum at 74 m^3.
Comparing with the results in figure 40, where the scenarios are similar except for the year, we can see that there is a fall in the LCOE. This means that as the years progress and the renewable penetration is as expected, hydrogen can be provided at a lower cost per kg than today. The Windshare(Windandteil) and Greenshare (Grünanteil) have also increased. This is due to the predicted increase in renewable penetration.

Scenario	Operation	Comb. Price	75% RE - Var. Storage
	Taxes	Reduced	Reduced
	Year	2030	2030
LCOE	€/MWh	159.06	141.75699
	€/Kg	5.297	4.72050777
PS (€)		32	70
PC (€)		34	70
Storage (m^3)		92	70
Green Share		0.64323205	0.63
Wind Share		0.35719159	0.35719159
Full load hours (ELY)		6334.9893	6334.9892
Efficiency (%)		0.53925101	0.53235562
Storage Cycles		302.02994	208.81359

Figure 42: Result - 2030 Reduced tax

In figure 42, you can see the results for the year 2030 where the tax is reduced. It can be seen that the LCOE is significantly lower in both the operating strategies when compared to the full tax scenario. This follows the trend observed in the year 2014. Here the PS and PC are 32€and 34 €. With a storage size of 92 m^3, which is the maximum allowed size with restriction, the smaller PS and PC are compensated with increased storage usage. With var. storage, the PS and PC are equal at 70 €. Here the storage cycles are lesser compared to the comb. price operating mode. This is because of the high and same PS and PC that the system operates in on-off mode. The optimum storage size is also smaller and estimated to be 70 m^3.

Scenario	Operation	Comb. Price	75% RE - Var. Storage
	Taxes	Free	Free
	Year	2030	2030
LCOE	€/MWh	149.89	149.89359
	€/Kg	4.991	4.99145655
PS (€)		32	32
PC (€)		34	34
Storage (m^3)		92	92
Green Share		0.64323205	0.66
Wind Share		0.35719159	0.35719159
Full load hours (ELY)		6334.9893	6334.9893
Efficiency (%)		0.53925101	0.53925101
Storage Cycles		302.02994	302.02994

Figure 43: Result - 2030 tax Free

The figure 43 shows the tax free scenario for the year 2030. It is interesting to note that the optimization tool box estimates the exact same values for the KPIs being considered to compare. This means that the optimum values are the same and that the effect of removing the restriction on the storage does not affect the optimum point.

With the var. storage operational strategy for 2030, a 75% renewable constraint is placed whereas in the 2014 scenario, a 50% renewable constraint is placed. This is an estimation as a 75% condition seems more logical for the year 2030 as the penetration of renewables in power production is expected to increase.

7.2.3 Year 2050

Similar to the year 2030, the predicted wind and green share for the years 2050 is used as input. The results from the simulation are shown below and discussed.

Scenario	Operation	Comb. Price	95% RE - Var. Storage
	Taxes	full	full
	Year	2050	2050
LCOE	€/MWh	249.26	248.28887
	€/Kg	8.300	8.26801937
PS (€)		70	51
PC (€)		70	64
Storage (m^3)		82	74
Green Share		0.90141177	0.90141177
Wind Share		0.50465918	0.50465918
Full load hours (ELY)		6334.9893	6334.9893
Efficiency (%)		0.53234681	0.53237053
Storage Cycles		178.21373	207.32365

Figure 44: Result - 2050 Full tax

The figure 44 shows the results from the simulations for the year 2050 where the tax is full. It can be seen that the LCOE is 8.30 €/kg for comb. price operation strategy and 8.26 €/kg for the var. storage. The normal trend observed in the previous year is not seen her. This can be because the removal of restriction on the storage size will give the optimizer a bit more freedom to optimize. Also it can be seen that the storage cycles are also increased.
Comparing with the results from the year 2030, there is a slight increase in the LCOE. Also it can be observed that the system operates in the on-off mode.

Scenario	Operation	Comb. Price	95% RE - Var. Storage
	Taxes	Reduced	Reduced
	Year	2050	2050
LCOE	€/MWh	141.46	141.46437
	€/Kg	4.711	4.71076352
PS (€)		70	70
PC (€)		70	70
Storage (m^3)		87	87
Green Share		0.90138758	0.89
Wind Share		0.5045822	0.51
Full load hours (ELY)		6334.9892	6334.9892
Efficiency (%)		0.5323399	0.5323399
Storage Cycles		167.98615	167.98615

Figure 45: Result - 2050 Reduced tax

Figure 45 shows the results from 2050 with reduced tax scenario. It can be seen that the LCOE is significantly lower compared to the full tax scenario and this follows the trend observed in the previous years considered. Comparing the LCOE with 2030 specifically, it can be observed that the LCOE is lower but not in a magnitude that is large enough to demand significant attention to this difference. This can be due to various factors like more renewables in the grid, change in way the system is operating, etc.

Comparing the comb. price and var. storage operation in the same year as shown in figure 45, it can be seen that the values are exactly same. This means that the maximum possible optimization has already been achieved even with restrictions on storage.

Scenario	Operation	Comb. Price	95% RE - Var. Storage
	Taxes	Free	Free
	Year	2050	2050
LCOE	€/MWh	132.27	131.07412
	€/Kg	4.405	4.3647682
PS (€)		70	51
PC (€)		70	64
Storage (m^3)		87	74
Green Share		0.90138758	0.90138758
Wind Share		0.5045822	0.5045822
Full load hours (ELY)		6334.9892	6334.9893
Efficiency (%)		0.5323399	0.53237053
Storage Cycles		167.98615	207.32365

Figure 46: Result - 2050 tax Free

The figure 46 shows the results for a tax free scenario. The LCOE is 4.40 €/kg for the comb. price and 4.36 €/kg for the var. storage operation strategy respectively. This can be explained in the same way as the previous case. Comparing these with reduced tax case for the same year, there is a reduction in the LCOE too.

7.3 Path 2 Results

The simulation results for path 2 for scenarios shown in table 4 are discussed here. The parameters that are discussed for this path are the the LCOE, LCOE of PV system (PVLCOE), Wind LCOE (WLCOE), Wind$_{usgage}$, PV$_{usgage}$ and efficiency (wirkungsgrad(%)).
The LCOE as discussed earlier will provide a flat platform to compare the scenarios. Wind and PV utilization gives us information on how much of electricity comes from them respectively in relation to the total energy used [13].

[13] Refer section 7.1.

Variables		Scenario 1
LCOE	€/MWh	199.10
	€/Kg	6.636
WLCOE	€/MWh	64.19
PVLCOE	€/MWh	123.88
Wind_usage (%)		0.92
PV_usage (%)		0.93
Efficiency (%)		0.53
Full load hours (ELY)		4265.39
Storage Cycles		3.08

Figure 47: Result - Path 2 - Scenario 1

Figure 47 shows the result from the simulation. This scenario is for Berlin and there is no restriction on the size of the wind renewable energy park. As you can see, The LCEO is 199.10 €/MWh. The wind LCOE is 64.19 €/MWH and PV LCOE is €/MWh. As seen in the previous pathway a standard electrolyser is used and the efficiency is 53%. It is interesting to note that the utilization of electrolyser can be seen from the full load hours (VLS_Ely). The value of 4265.39 h/a is not that high which means the electrolyser is not being used that much. It is more interesting to see that the full load cycles (VLSpeicherzyklen) is around 3. This means only approximately 3 times the entire storage capacity of the cavern is being used the entire year. This can signify that the demand for hydrogen is met on a more daily basis. Based on the impact of investment cost of the cavern on the LCOE (refer section 7.4.2), decisions can be made or reducing the cavern volume so that it is used for more cycles.

Variables		Scenario 2
LCOE	€/MWh	203.25
	€/Kg	6.774
WLCOE	€/MWh	61.23
PVLCOE	€/MWh	120.22
Wind_usage (%)		0.97
PV_usage (%)		0.97
Efficiency (%)		0.53
Full load hours (ELY)		3792.96
Storage Cycles		3.01

Figure 48: Result - Path 2 - Scenario 2

The results for the scenario 2 can be seen in figure 48. Comparing the previous scenario, it can be seen that the LCOE has increased to 203.25 €/MWh. This is because there is a restriction placed on the size of renewable energy park. The wind and PV LCOEs have reduced marginally. This can be explained by their increased utilization. The efficiency of the system is still the same at 53 % and it is interesting to note that the full load hours of the electrolyser has been reduced. This can be because the optimizer thinks that this is the right amount of full load hours that can result in the lowest LCOE. The Full load storage cycles are also almost the same as in previous scenario.

Variables		Scenario 3
LCOE	€/MWh	224.31
	€/Kg	7.476
WLCOE	€/MWh	63.47
PVLCOE	€/MWh	121.50
Wind_usage (%)		0.93
PV_usage (%)		0.94
Efficiency (%)		0.53
Full load hours (ELY)		3930.25
Storage Cycles		3.31

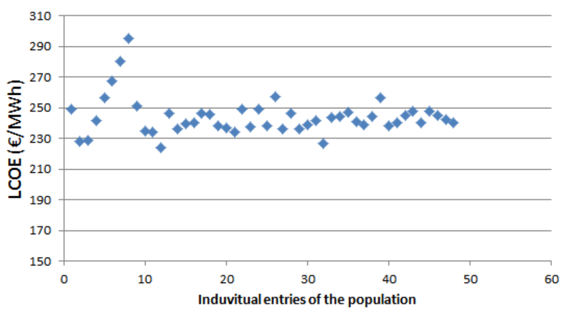
Figure 49: Result - Path 2 - Scenario 3

Figure 49 shows the results from the scenario 3. Here u can see that the LCOE has further increased to 224.31 €/MWh. This is because, in this scenario the renewable energy park is far from the industry which requires the produced hydrogen. This brings in additional costs into the scenario due to pipelines and also buffer storages are used to maintain the minimum input/output rates to the cavern. There is marginal increase in the wind and PV LCOEs too. There is increased use of electrolyser compared to scenario 2 but it is still less than that of scenario 1. The Full load storage cycles are highest seen so far in this path, but still in the same range. The wind$_{usage}$ and PV$_{usage}$ are at 93% and 94% respectively.

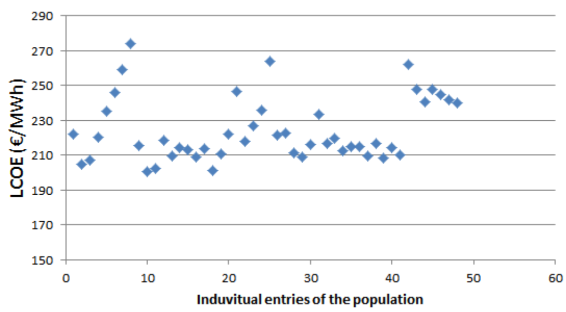
Variables		Scenario 4
LCOE	€/MWh	200.55
	€/Kg	6.684
WLCOE	€/MWh	64.19
PVLCOE	€/MWh	123.88
Wind_usage (%)		0.92
PV_usage (%)		0.93
Efficiency (%)		0.53
Full load hours (ELY)		4265.39
Storage Cycles		3.08

Figure 50: Result - Path 2 - Scenario 4

In scenario 4, a longer pipeline than that of scenario 3 is assumed. It is important to do this because for transporting hydrogen over longer distances, intermediate compressor stages are necessary to maintain the pressure [46]. So this must add investment cost and operating costs. This should increase the LCOE compared to scenario 3 but the LCOE is reduced to 200.55 €/MWh. This can be because the introduction of compressor and its associated variables provides the optimizer new optimization points. This can be seen from figure 51that the data set is more spread out.



(a) Scenario 3



(b) Scenario 4

Figure 51: Data set for optimization - LCOE

The Full load hours is similar to scenario at 4265.39 h/a.

Variables		Scenario 5
LCOE	€/MWh	198.72
	€/Kg	6.623
WLCOE	€/MWh	61.23
PVLCOE	€/MWh	120.22
Wind_usage (%)		0.97
PV_usage (%)		0.97
Efficiency (%)		0.53
Full load hours (ELY)		3792.96
Storage Cycles		3.01

Figure 52: Result - Path 2 - Scenario 5

Figure 52 shows the results from scenario 5. The end users here are the mobility sector. Here the gas demand from the industry is set to zero and the demand curves of a mobility sector as explained in the section 6.4.1 is used. It is interesting to see that the LCOE is in a similar range compared to scenario 1 of path 2. The LCOE value is 198.72 €/MWh. The wind and PV LCOEs are at 61 €/MWh and 120.22 €/MWh respectively. The wind and PV utilization are high at 97%.

Variables		Scenario 6
LCOE	€/MWh	203.25
	€/Kg	6.774
WLCOE	€/MWh	61.23
PVLCOE	€/MWh	120.22
Wind_usage (%)		0.97
PV_usage (%)		0.97
Efficiency (%)		0.53
Full load hours (ELY)		3792.96
Storage Cycles		3.01

Figure 53: Result - Path 2 - Scenario 6

Scenario 6 is similar to that of the previous one apart from the fact that there is a restriction on the size of the wind park. This results in a marginal increase of LCOE. The other parameters pretty much remain the same. What would be more interesting would be do these simulation for another location. The type of the location can be anything varying from a pure wind site with no PV and vice-versa.

7.4 Sensitivity Analysis

The sensitivity analysis is used to get an insight into how a change in one of the variables affect the LCOE of the final hydrogen produced. The analysis is done in MATLAB.

The model used for the sensitivity analysis is similar to the model used for the optimization earlier. A variable named **Sensi** is created and given values ranging from 0.6 to 1.5 with steps of 0.1 (10 values). This variable is then multiplied with the parameter for which the analysis is being done. The parallel computing toolbox is used and 10 sets of start up population is created, each with one value of Sensi variable multiplied with the parameter being considered. The calculations are done and complied together which gives us information on how much variation is caused in the LCOE by changing the value of the parameter being considered.

7.4.1 Path 1

The parameters that are chosen to be used for the sensitivity analysis is based on the scenario. For Path 1 the following parameters are chosen for sensitivity analysis:-

- Investment cost of Electrolyser
- Investment cost of Storage tank
- Investment cost of stack
- Operating cost of Electrolyser
- Operating cost of Storage tank
- Lifetime of Stack.

Investment costs play a major role in the calculation of LCOE and hence it was chosen. Stacks, Electrolyser and the storage being some of the most important components with high investment costs, their investment costs are chosen specifically for the analysis. Their operating costs are also considered as it gives a good insight into the how the working of the plant would affect the costs and hence the LCOE. The lifetime of the stacks are also important as with advanced in technology, it is possible that stacks with higher lifetimes than today would be developed. It would be interesting to know how much this would affect the LCOE today and in future.

Figure 54 shows the results from the sensitivity analysis for the reference year 2014 where there is full tax on the electricity consumed from the grid. The results have be converted to a graphical format for easier understanding.

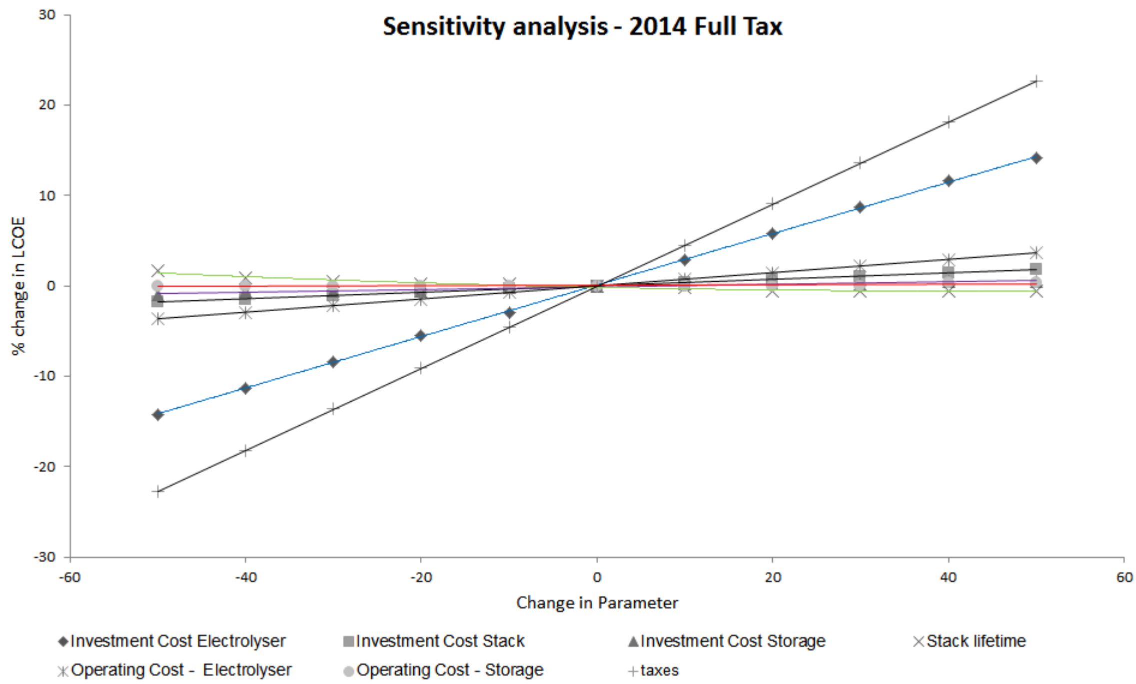


Figure 54: Sensitivity analysis - 2014 - Full Tax

It can be seen that there is a big impact on the LCOE by the Investment cost - Electrolyser. But the biggest impact is from the taxes. A small change in the tax produces a significant change in the LCOE compared to the other parameters. Als the nature of the impact is different depending on the parameter. As seen in figure 54, increase in running cost of electrolyser and storage has a different effect compared to the increase in investment cost of electrolyser. This is because an increase in operating costs shows that more usage of storage and electrolyser is being done which reduces the overall LCOE.

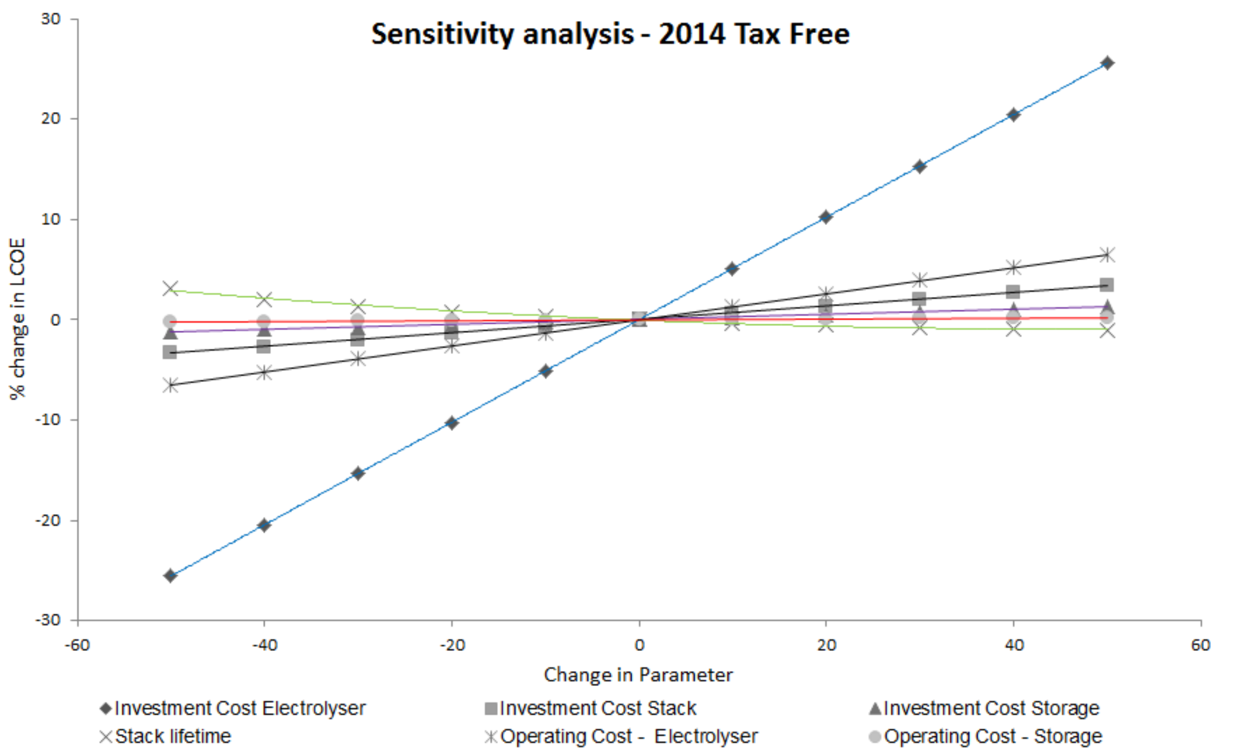


Figure 55: Sensitivity analysis - 2014 - Reduced Tax

Figure 55 shows the sensitivity analysis for the scenario in 2014 where there is no tax. It can be seen that now the impact of change in investment cost of electrolyser is greater than in the previous case. This is because the effect of electricity price is reduced in this scenario and that in turn increases the effect of electrolyser investment cost.

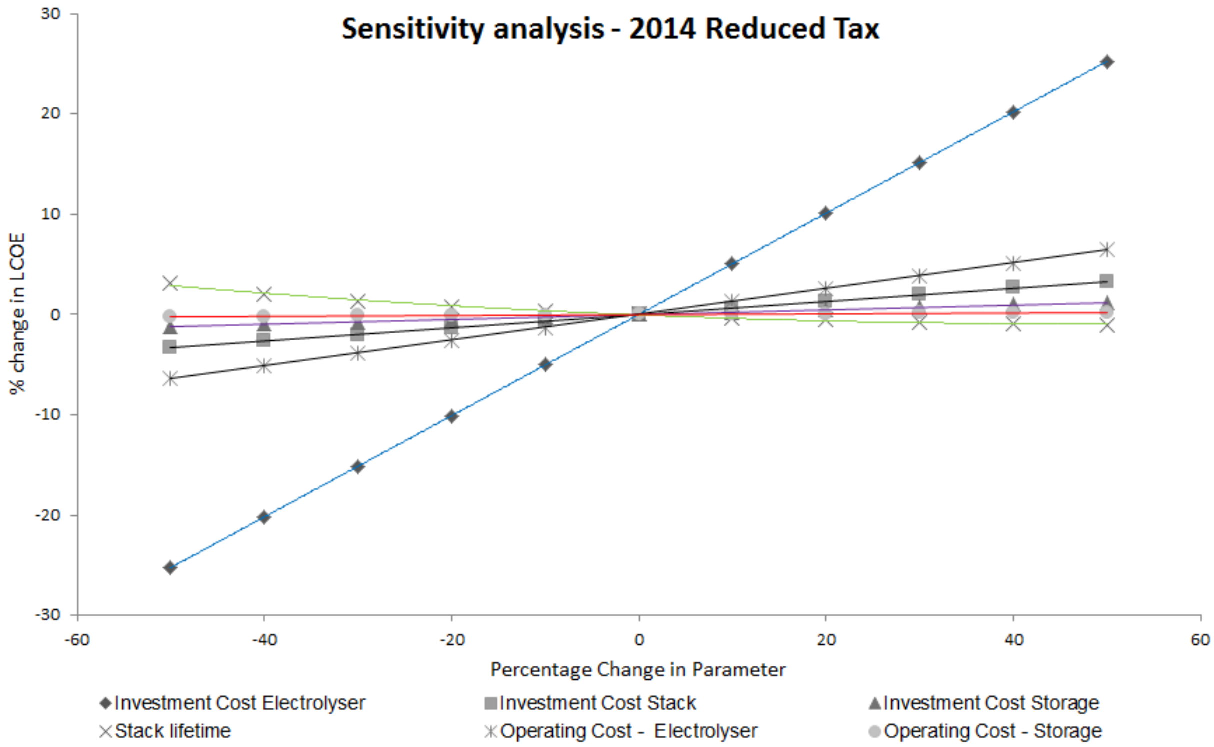


Figure 56: Sensitivity analysis - 2014 - Tax Free

Figure 56 is similar to the previous scenario with free tax. This is because a discount in the price of the electricity based on consumption is done at 1GWh. The actual consumption is way higher than this cap and hence the effect of reduced tax does not play a significant difference when compared with a tax free scenario.

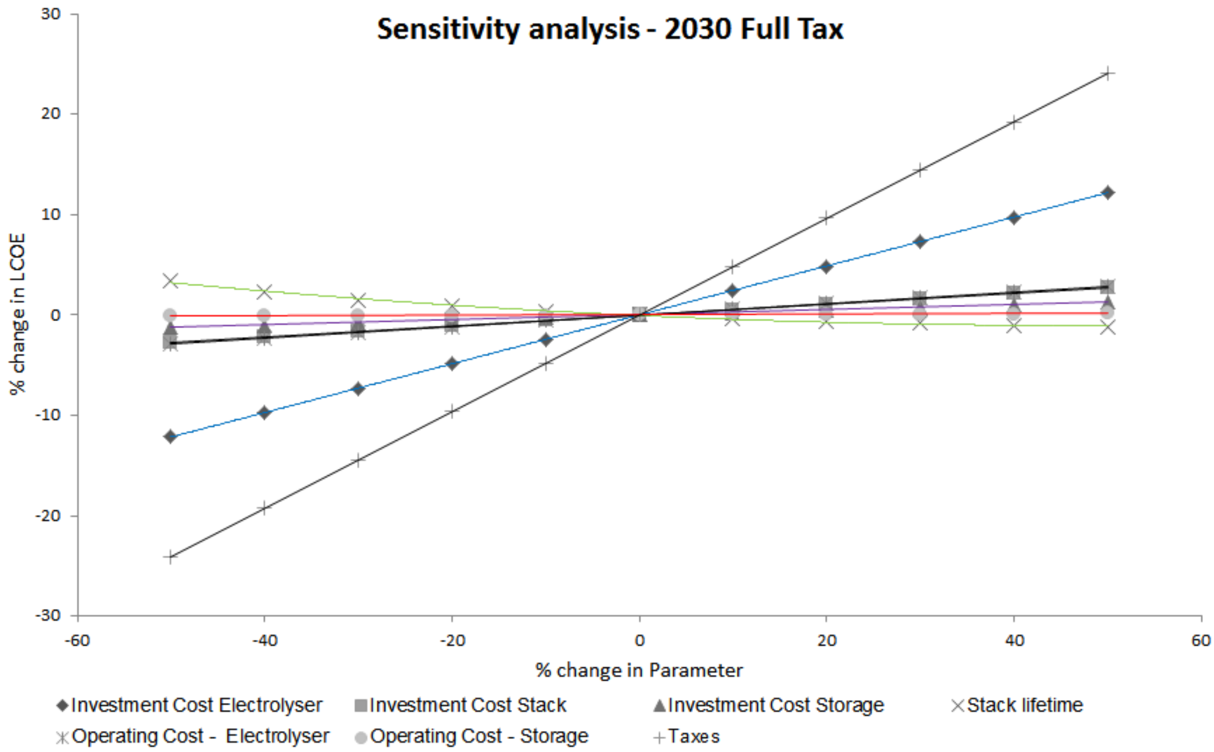


Figure 57: Sensitivity analysis - 2030 - Full Tax

Figure 57 shows the graph of the parameters considered for the year 2030. It can be seen that the impact of investment cost of the electrolyser has significantly reduced. This can be attributed to the reduction in prices of electrolyser and that the technology is developing every year drastically with advances in material science and other related fields. The impact of operation cost of the storage almost negligible. Although, Compared to the year 2014, it can be seen that the investment cost of storage has a greater impact. Also the taxes are the biggest impact here. This follows the trend seen in figure 54 for the year 2014. Reduction in the taxes/duties will lower the LCOE by a large amount.

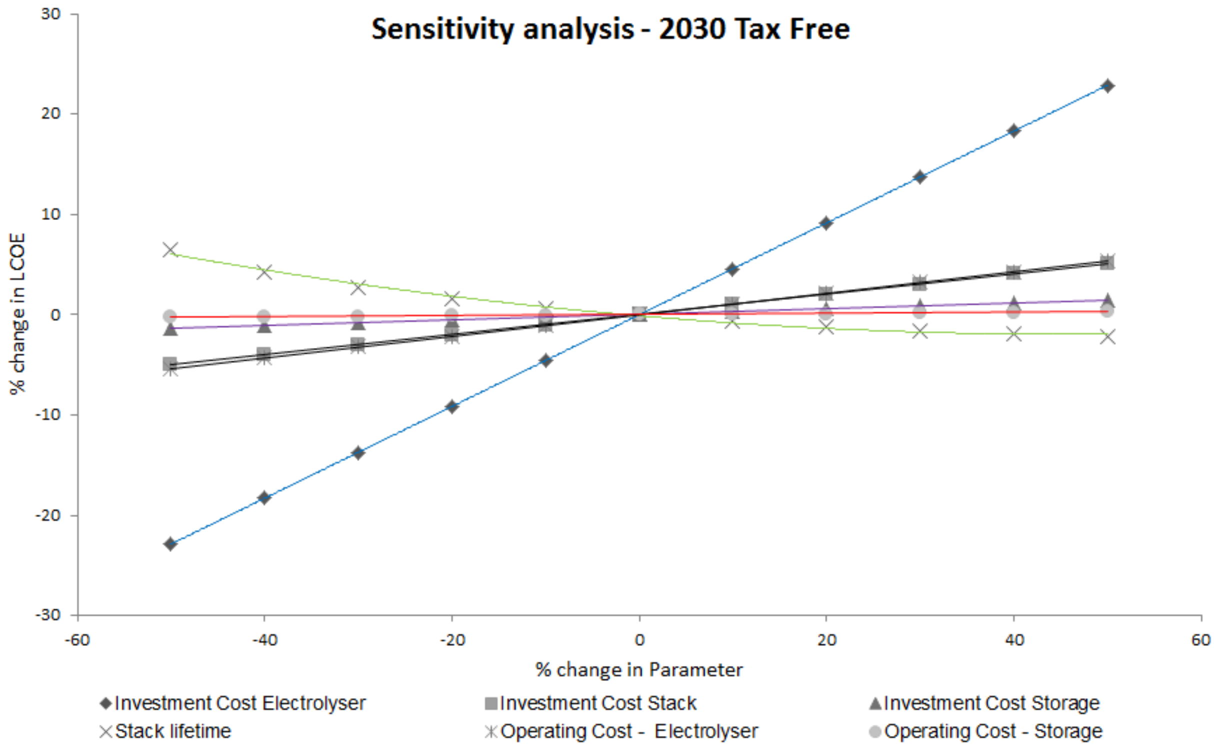


Figure 58: Sensitivity analysis - 2030 - Reduced Tax

The scenario for the year 2030 without any tax is shown in figure 58. With the price of electricity being relatively cheaper now, the impact of investment cost of electrolyser is higher than in the scenario shown in figure 57. Also it is interesting to see that different impact the parameters have on the LCOE. Clearly the impact of Stack lifetime (green line) and the investment cost of electrolyser (blue line) are different. This is understandable as increasing the life time of the stack means lesser investment per year and this means the LCOE decreases.

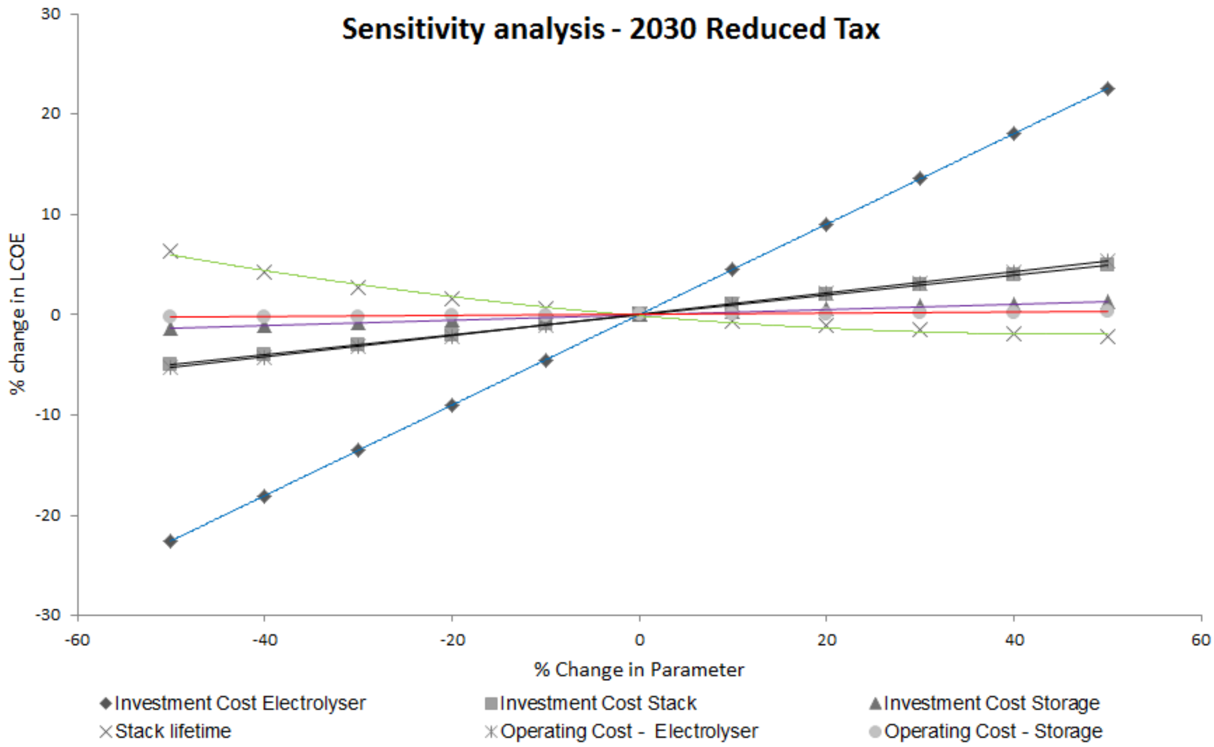


Figure 59: Sensitivity analysis - 2030 - Tax Free

As it is in the case of previous scenarios, there is very little difference in the impact of parameters on the LCOE when comparing between the reduced tax and tax free scenarios. The variations are in the order of 10^{-2} which is insignificant to be able to visually see it in the graph considering the scale that has been used. The values based on which the graphs have been drawn can be seen in appendix section at the end of this thesis.

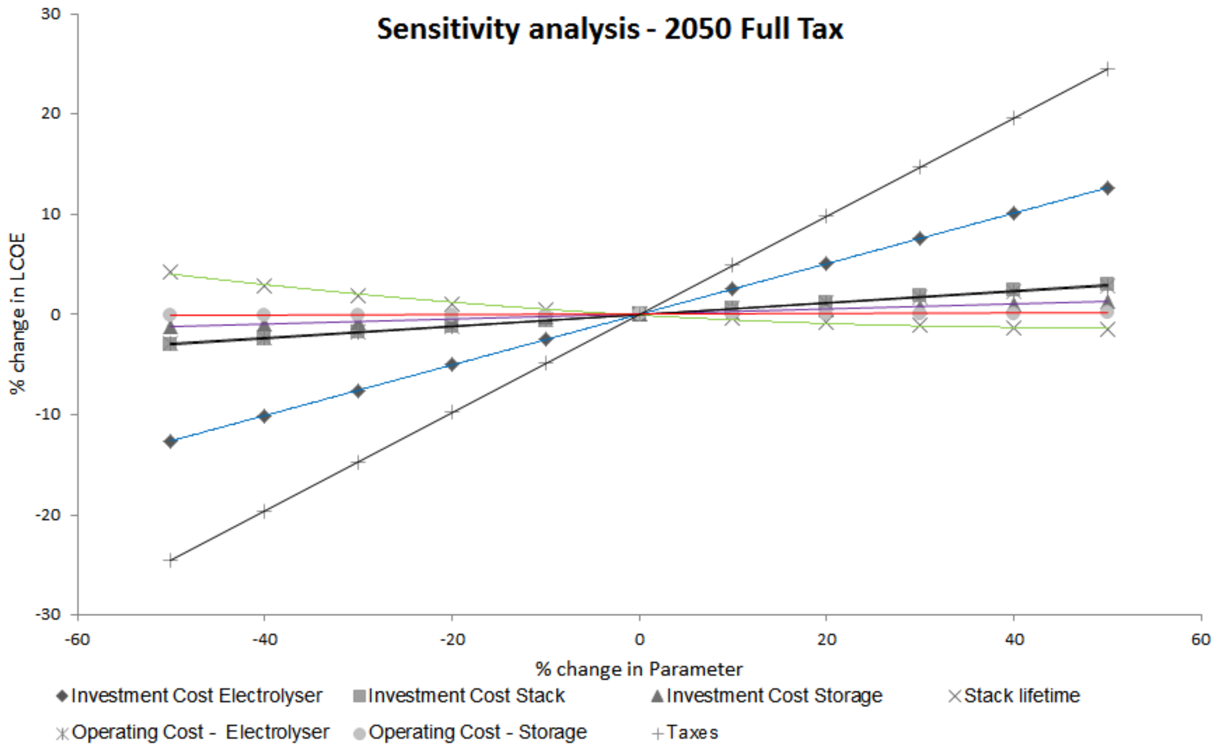


Figure 60: Sensitivity analysis - 2050 - Full Tax

Figure 60 shows the sensitivity analysis done for the year 2050 without any subsidy from the government. This represents a fully taxed scenario. It can be seen that the impact of the variables are similar to that in the year 2030. But it is also important to note that there is a slightly increased impact on the LCOE [14]. This can be due to the maturing of technology by 2050. Also similar to the previous two years, the impact of taxes/duties is the highest. This further emphasises the importance on the role that can be played by the government in lowering the taxes so that the hydrogen can be provided at lower prices.

[14] Refer section A.1 for accurate values

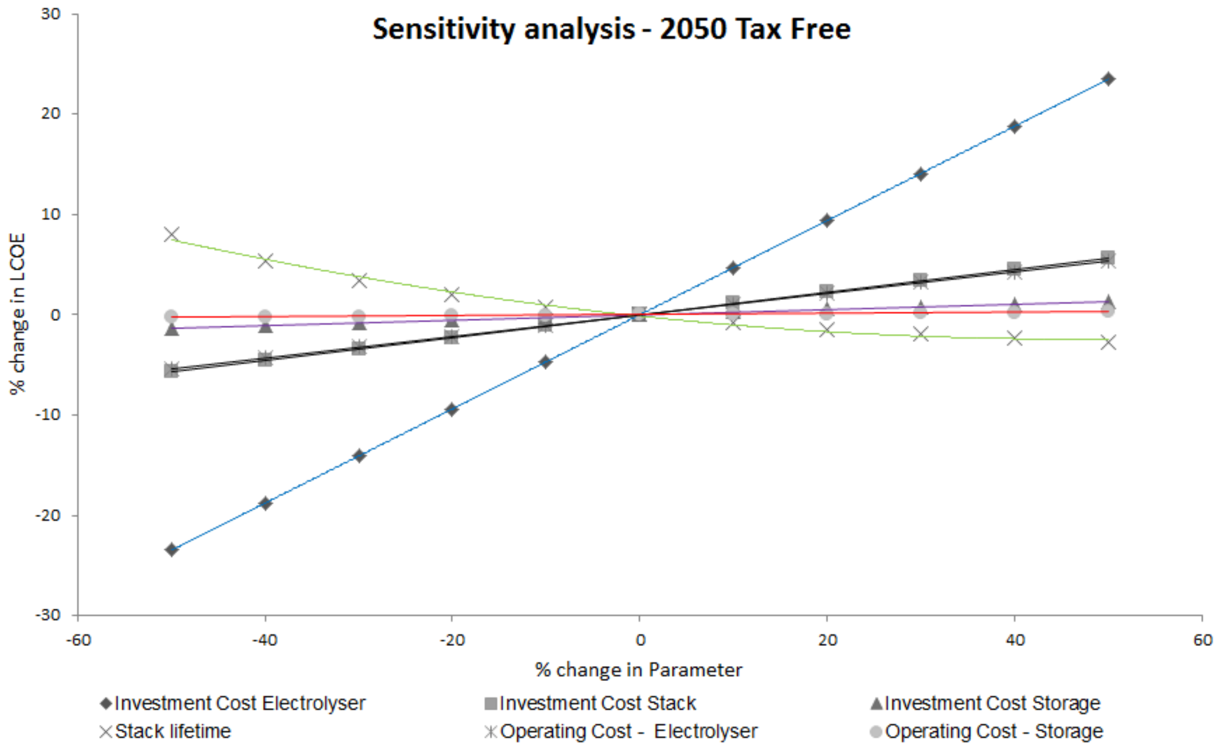


Figure 61: Sensitivity analysis - 2050 - Reduced Tax

The tax free scenario for 2050 is shown in figure 61. This when compared to the full tax scenario of the same year, it can be seen that the influence of changing investment cost of electrolyser is higher. This can be understood as the electricity is cheaper no due to the absence of tax, there is much more influence on the LCOE by the investment cost of electrolyser and stack.

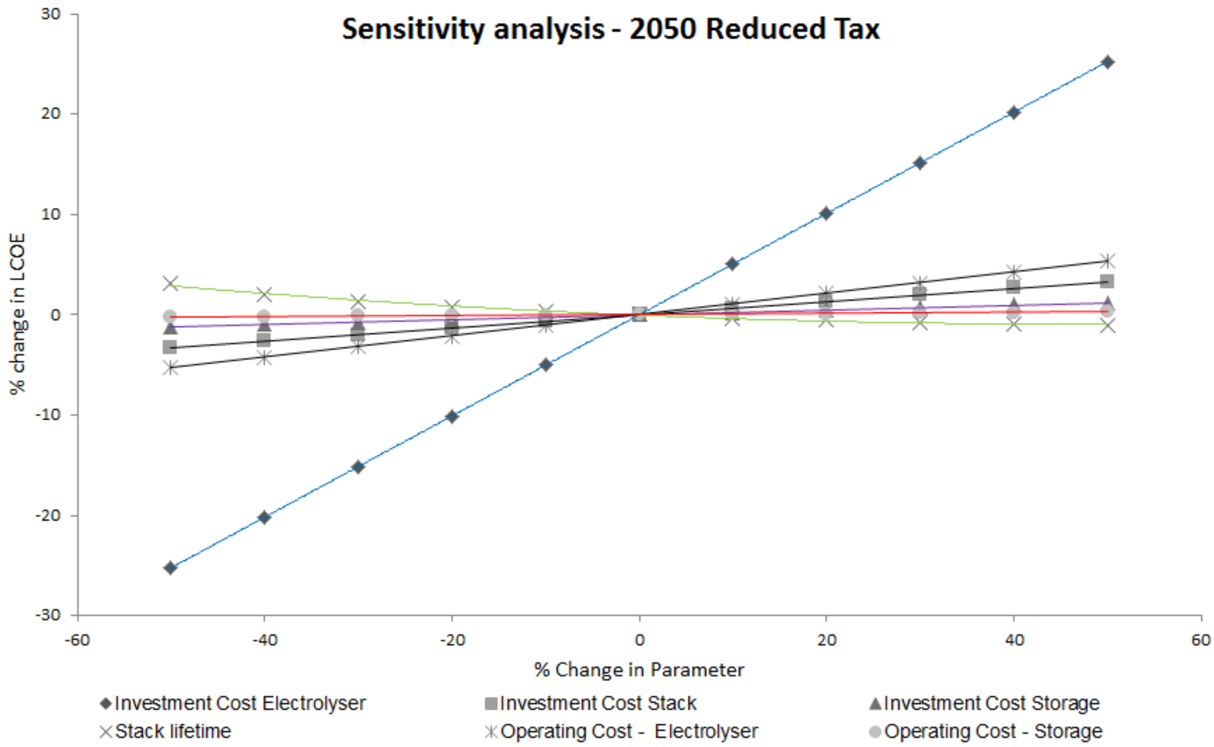


Figure 62: Sensitivity analysis - 2050 - Tax Free

As seen from the previous scenarios, there is not much difference in the influence of parameters on the LCOE compared to the tax free scenario. But this would be interesting to know as this might be the next step from a fully taxed scenario, providing marginal benefit to the policy makers but still making good use of the electricity to give hydrogen at low prices.

7.4.2 Path 2

Similar sensitivity analysis was carried out for the second path too. Unlike path 1, the analysis is not carried out for every path. This is because the parameters changing between the scenarios in this case does not affect the system dynamically. For example, between scenarios 1, 2 and 3 in the first path, the taxes/duties were the difference. This affects the price of the electricity taken from the grid throughout the simulation. Whereas, the difference between the scenarios here are going to produce a one-off impact. Hence only one sensitivity analysis was done to see the effects of parameters of interest. The methodology of the analysis is itself same although parallel computing was not used here.

The following parameters were chosen for the analysis sensitivity analysis in this path.

- Investment Cost - Cavern
- Investment Cost - Electrolyser
- Lifetime - Cavern
- Lifetime - PV
- Operating Costs - Cavern
- Operating Costs - Wind
- Operating Costs - PV

The investment cost of the Cavern and electrolyser are important as this would directly have a big impact on the electrolyser. It would be interesting to know the impact of cavern investment cost on the LCOE as cavern storage is stil developing and potentially the costs would reduce in future. Operating costs of wind, pv and cavern are considered for the sensitivity analysis too.

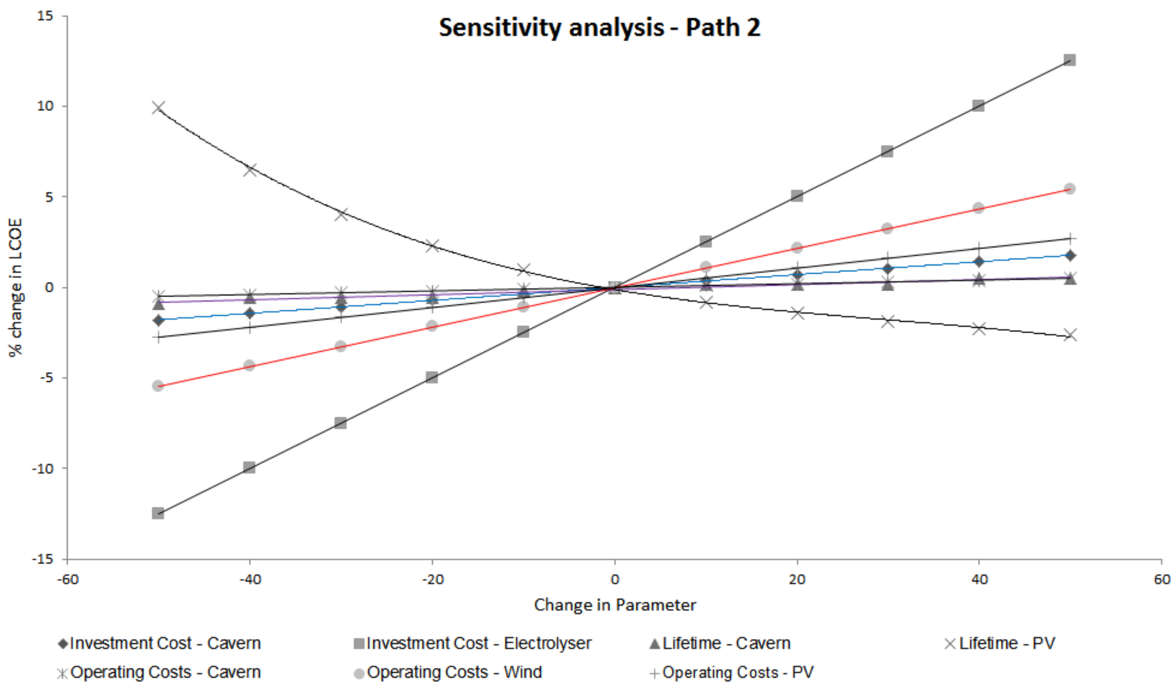


Figure 63: Sensitivity analysis - Path 2

Figure 63 shows the results of the sensitivity analysis for path 2. Here it is easy to see that the investment cost of the electrolyser has the biggest impact. A change of 10% creates a change of around 2.5% in the LCOE [15].

Wind operating costs also have an observable impact. As expected increasing the operating costs of wind park increases the LCOE. Logically this makes sense and reducing the operating costs would be one of the ways to reduce the LCOE. Similarly, the PV operating costs also have the same kind of impact althought not on the same scale. This is because the operating costs of PV is less compared to its overall costs [47].
The operating cost of cavern has very little impact on the LCOE. This is because the cavern has very minimal operational costs. Investment cost of the cavern has an impact that is expected of it. Lowering the investment cost of the cavern does reduce the LCOE. This can provide some opportunities for reduction of LCOE as advances in research in the field of material science will reduce the investment costs in future.
The only anomaly the can be is the impact of life time of PV. Increasing the lifetime of any investment actually will lead to reduced investment per year. This should technically reduce the LCOE, but here the opposite is observed. This can be because of some error with the optimization.

[15] Refer section A.2 for exact values

8 Conclusion

Analysis on the scenarios were done and some interesting results were found.

The most interesting finding is the influence of taxes on the LCOE in the first scenario. Section 6.5 explained how the taxes are fixed and why they are being charged. Based on the result below from the sensitivity analysis for the scenario 2014 with taxes, the impact can be clearly seen.

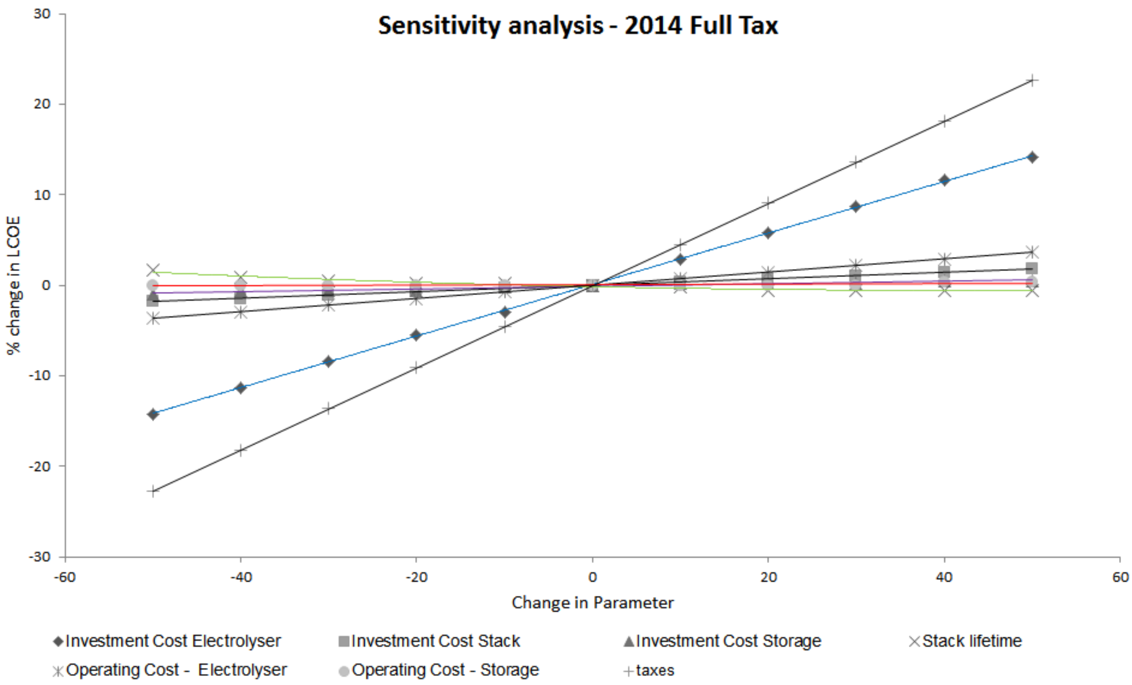


Figure 64: Sensitivity analysis - Full Tax

It is clear that the taxes are the biggest impact and this can be seen not only in the year 2014 but also for the simulated results for the years 2030 and 2050. This clearly puts a perspective on what can be done by the government in the field of P2G. Investment costs operating costs and other factors all do can contribute to reducing the LCOE but these are based on how much scientific advancements can be made in future. There is a certain degree of uncertainty there. But with respect to taxes, it can be clearly seen that if the predicted pattern of power production and renewable penetration continues, then the government policy changes can produce the biggest impact in reducing the costs at which hydrogen can be produced and offered.

9 Outlook

For the accuracy of the results, real life scenario has be depicted as much as possible by using a variety of inputs. Also, during the course of this thesis, some assumptions have been made to make the computation as fast as possible. This gives us a picture close to how things would happen real life. There are other improvements that can be done to improve the accuracy of the results.

For example a simple electrolyser has been considered for both the pathways. There are different types of electrolysers that can be used. For example, model of the electrolyser are based on a standard system. These systems do not operate under overload conditions the rate of hydrogen production is not the best in the market. These offer a good combination of production rate, efficiency, lifetime and reasonable investment cost. On the other hand a high performance system can also be used. A high performance system can be operated when the electricity cost is high but the demand for hydrogen makes it necessary for the production of hydrogen. At this juncture, a high performance system would yield more hydrogen which can potentially reduce the LCOE. It is important to note that the investment in this case would be higher than a standard system and hence more analysis must be done to see how much of an advantage it can be to use a high performance system.

Also there are systems with overload capabilities. This can be an option when a high performance system is too expensive. With a system with overload capabilities, when the electricity prices are lower, it can be run above its rated power and produce more hydrogen. This can reduce the LCOE.
In the second path, it was observed that for almost all the scenarios, the full load storage cycles were around 3. This means that only 3 times the volume of the designated storage size was used the entire year. This points to the fact that the necessity of storage is lesser in this path. The optimization can be carried out futher allowing the optimization tool box to find out an optimum storage size like in the simulations for path 1.

Also, the wind to PV ratio was always maintained at 1:1 for the second path. This is based on the assumption that the site chosen is equally good for wind and PV. In reality there might be places that are more suitable for wind and less suitable for PV or the other way around. So the simulation can be done allowing the optimization to find a suitable ratio between wind and PV investment. This will take longer computational times, but will give results that are worth understanding.

Building upon this, simulations can be carried out for locations in northern europe where the location is primarily suitable for wind. It might be possible that just a wind renewable energy park might be enough to provide all the necessary hydrogen demand by the industry or the mobility sector.

All these above suggestion are meant to provide an outlook into what can be done further to understand better the possibility of P2G pathways being the backbone of mobility sector and possibly the industry. It is an undeniable fact that this technology provides the best balance between bridging the gap between an intermittent energy source and a highly dynamic demand side. It is clearly evident that renewables are going to occupy a bigger share in the amount of energy produced and this emphasis more on the need for not just better storage options but dynamic control in the deployment of stored energy.

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A Appendix

A.1 Sensitivity analysis - Path 1

2014 - Full Tax

% change in parameter	% change in LCOE: Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-14.18181818	-1.818181818	-0.907441016	1.633394	-3.636363636	0
-40	-11.27272727	-1.454545455	-0.54446461	0.907441	-2.909090909	0
-30	-8.363636364	-1.090909091	-0.54446461	0.544465	-2.181818182	0
-20	-5.454545455	-0.727272727	-0.54446461	0.181488	-1.454545455	0
-10	-2.909090909	-0.363636364	-0.181488203	0.181488	-0.727272727	0
0	0	0	0	0	0	0
10	2.909090909	0.363636364	0.181488203	-0.18149	0.727272727	0
20	5.818181818	0.727272727	0.181488203	-0.54446	1.454545455	0
30	8.727272727	1.090909091	0.181488203	-0.54446	2.181818182	0
40	11.63636364	1.454545455	0.54446461	-0.54446	2.909090909	0.363636364
50	14.18181818	1.818181818	0.54446461	-0.54446	3.636363636	0.363636364

2014 - Tax Free

% change in parameter	% change in LCOE: Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-25.55354432	-3.346087832	-1.247641934	3.108584	-6.505246978	-0.248072593
-40	-20.44283871	-2.676868311	-0.998116804	2.06046	-5.20419628	-0.198458074
-30	-15.33212659	-2.007655304	-0.748585161	1.312364	-3.903152095	-0.148843556
-20	-10.22142098	-1.338435784	-0.499060031	0.751795	-2.602101397	-0.099229037
-10	-5.110708864	-0.669216264	-0.249528387	0.316229	-1.301050698	-0.049614519
0	0	0	0	0	0	0
10	5.110708864	0.669216264	0.249528387	-0.31623	1.301050698	0.049614519
20	10.22141447	1.33842927	0.499053517	-0.55291	2.602101397	0.099229037
30	15.33212659	2.007648791	0.748585161	-0.75288	3.903152095	0.148843556
40	20.4428322	2.676868311	0.998110291	-0.92399	5.204202793	0.198458074
50	25.55354432	3.346081318	1.247635421	-1.07203	6.505253492	0.248072593

2014 - Reduced Tax

% change in parameter	% change in LCOE: Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-25.23293645	-3.304106097	-1.231988379	3.069595	-6.42362881	-0.244960147
-40	-20.18635237	-2.643282948	-0.985593919	2.034617	-5.138901762	-0.195968117
-30	-15.13976187	-1.982466231	-0.739193027	1.295904	-3.854181145	-0.146976088
-20	-10.09317779	-1.321643082	-0.492798567	0.742365	-2.569454097	-0.097984059
-10	-5.046587289	-0.660819933	-0.246397676	0.312262	-1.284727048	-0.048992029
0	0	0	0	0	0	0
10	5.046587289	0.660819933	0.246397676	-0.31226	1.284727048	0.048992029
20	10.09317136	1.32163665	0.492792136	-0.54598	2.569454097	0.097984059
30	15.13976187	1.982459799	0.739186595	-0.74343	3.854181145	0.146976088
40	20.18634594	2.643282948	0.985587487	-0.9124	5.138908194	0.195968117
50	25.23293645	3.304099665	1.231981947	-1.05858	6.423635242	0.244960147

2030 - Full Tax

% change in parameter	% change in LCOE					
	Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-12.30769231	-2.682095993	-1.272518624	3.440583	-2.865353349	-0.146442469
-40	-9.615384615	-2.145677948	-1.018011577	2.280514	-2.292283833	-0.117154359
-30	-7.307692308	-1.609259903	-0.763511174	1.452526	-1.719214317	-0.08786625
-20	-5	-1.072838013	-0.509004128	0.832084	-1.146140955	-0.058578141
-10	-2.307692308	-0.536419968	-0.254503725	0.350006	-0.573071439	-0.029290032
0	0	0	0	0	0	0
10	2.307692308	0.536419968	0.254503725	-0.35001	0.573071439	0.029290032
20	5	1.072838013	0.509004128	-0.61196	1.146140955	0.058578141
30	7.307692308	1.609259903	0.763511174	-0.83328	1.719214317	0.08786625
40	9.615384615	2.145677948	1.018011577	-1.02267	2.292283833	0.117154359
50	12.30769231	2.682095993	1.272518624	-1.18652	2.865353349	0.146442469

2030 - Tax Free

% change in parameter	% change in LCOE					
	Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-22.87241146	-5.041816517	-1.384468194	6.46562	-5.386304548	-0.275279609
-40	-18.297927	-4.033455382	-1.107576724	4.285593	-4.309045807	-0.220223687
-30	-13.72344977	-3.025087019	-0.830685253	2.729619	-3.231779838	-0.165167766
-20	-9.148965305	-2.016725884	-0.553786555	1.563671	-2.154521096	-0.110111844
-10	-4.574480846	-1.008364749	-0.276895084	0.657738	-1.077262355	-0.055055922
0	0	0	0	0	0	0
10	4.574480846	1.008364749	0.276895084	-0.65774	1.077262355	0.055055922
20	9.148965305	2.016733112	0.553793783	-1.15001	2.154528324	0.110111844
30	13.72344977	3.025094247	0.830685253	-1.56592	3.231787066	0.165167766
40	18.29793422	4.033455382	1.107576724	-1.92183	4.309045807	0.220223687
50	22.87241868	5.041823745	1.384475422	-2.22973	5.386311776	0.275279609

2030 - Reduced Tax

% change in parameter	% change in LCOE					
	Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-22.55440708	-4.971718106	-1.365219374	6.375785	-5.311416581	-0.271452286
-40	-18.04352353	-3.977376623	-1.092177637	4.226048	-4.249135403	-0.217161829
-30	-13.5326471	-2.983028013	-0.819135901	2.691692	-3.186847097	-0.162871371
-20	-9.021763546	-1.98868653	-0.546087037	1.541945	-2.12456592	-0.108580914
-10	-4.510879991	-0.994345047	-0.2730453	0.648599	-1.062284742	-0.054290457
0	0	0	0	0	0	0
10	4.510879991	0.994345047	0.2730453	-0.6486	1.062284742	0.054290457
20	9.021763546	1.988693657	0.546094164	-1.13403	2.124573047	0.108580914
30	13.5326471	2.98303514	0.819135901	-1.54416	3.186854225	0.162871371
40	18.04353066	3.977376623	1.092177637	-1.89513	4.249135403	0.217161829
50	22.55441421	4.971725234	1.365226501	-2.19875	5.311423708	0.271452286

2050 - Full Tax

	% change in LCOE					
% change in parameter	Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-12.62397881	-3.048777824	-1.246211387	4.3051	-2.885737717	-0.144673403
-40	-10.09918191	-2.439022259	-0.996971061	2.853543	-2.308590174	-0.115738723
-30	-7.574385008	-1.829266694	-0.74772423	1.817502	-1.73144263	-0.086804042
-20	-5.049591905	-1.21951113	-0.498483904	1.041163	-1.154295087	-0.057869361
-10	-2.524795003	-0.609755565	-0.249243579	0.437949	-0.577147543	-0.028934681
0	0	0	0	0	0	0
10	2.524795003	0.609755565	0.249243579	-0.43795	0.577147543	0.028934681
20	5.049591905	1.21951113	0.49849041	-0.76573	1.154295087	0.057869361
30	7.574388807	1.829266694	0.747730736	-1.04266	1.731438832	0.086804042
40	10.09918571	2.439022259	0.996977567	-1.27964	2.308586375	0.115738723
50	12.62397881	3.048777824	1.246217893	-1.48466	2.885733918	0.144673403

2050 - Tax Free

	% change in LCOE					
% change in parameter	Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-23.481312	-5.670899524	-1.353396135	8.004692	-5.36762862	-0.269100729
-40	-18.78505384	-4.536719619	-1.082719734	5.305737	-4.294108549	-0.215280583
-30	-14.08878861	-3.402539715	-0.812036268	3.379373	-3.220581412	-0.161460437
-20	-9.392523388	-2.26835981	-0.541359867	1.935885	-2.147054274	-0.107640291
-10	-4.696265227	-1.134179905	-0.270676401	0.814304	-1.073527137	-0.053820146
0	0	0	0	0	0	0
10	4.696265227	1.134179905	0.270676401	-0.8143	1.073527137	0.053820146
20	9.392523388	2.26835981	0.541359867	-1.42376	2.147054274	0.107640291
30	14.08878861	3.402539715	0.812036268	-1.93867	3.220581412	0.161460437
40	18.78505384	4.536719619	1.082719734	-2.3793	4.294108549	0.215280583
50	23.481312	5.670899524	1.353396135	-2.7605	5.36762862	0.269100729

2050 - Reduced Tax

	% change in LCOE					
% change in parameter	Investment Cost Electrolyser	Investment Cost Stack	Investment Cost Storage	Stack lifetime	Operating Cost Electrolyser	Operating Cost - Storage
-50	-25.23293645	-3.304106097	-1.231988379	3.069595	-5.294652635	-0.26544215
-40	-20.18635237	-2.643282948	-0.985593919	2.034617	-4.235727684	-0.21235372
-30	-15.13976187	-1.982466231	-0.739193027	1.295904	-3.176795763	-0.15926529
-20	-10.09317779	-1.321643082	-0.492798567	0.742365	-2.117863842	-0.10617686
-10	-5.046587289	-0.660819933	-0.246397676	0.312262	-1.058931921	-0.05308843
0	0	0	0	0	0	0
10	5.046587289	0.660819933	0.246397676	-0.31226	1.058931921	0.05308843
20	10.09317136	1.32163665	0.492792136	-0.54598	2.117863842	0.10617686
30	15.13976187	1.982459799	0.739186595	-0.74343	3.176795763	0.15926529
40	20.18634594	2.643282948	0.985587487	-0.9124	4.235727684	0.21235372
50	25.23293645	3.304099665	1.231981947	-1.05858	5.294652635	0.26544215

A.2 Sensitivity analysis - Path 2

	% change in LCOE						
% change in parameter	Investment Cost - Cavern	Investment Cost - Electrolyser	Lifetime - Cavern	Lifetime - PV	Operating Costs - Cavern	Operating Costs - Wind	Operating Costs - PV
-50	-1.782953561	-12.50422031	-0.907441016	9.937799	-0.482987303	-5.434162657	-2.737924603
-40	-1.426361485	-10.00337488	-0.54446461	6.467352	-0.386387114	-4.347331001	-2.190338807
-30	-1.069772819	-7.502532868	-0.54446461	4.0588	-0.289790335	-3.260499346	-1.642757389
-20	-0.713180742	-5.001687442	-0.54446461	2.31169	-0.193193557	-2.17366769	-1.095171593
-10	-0.356592077	-2.500845426	-0.181488203	1.00334	-0.096596778	-1.086836034	-0.547585796
0	0	0	0	0	0	0	0
10	0.356588665	2.500842015	0.181488203	-0.78355	0.096596778	1.086831656	0.547581418
20	0.713180742	5.001687442	0.181488203	-1.40418	0.193193557	2.173663312	1.095167215
30	1.069772819	7.502532868	0.181488203	-1.90131	0.289790335	3.260494968	1.642753011
40	1.426361485	10.00337488	0.54446461	-2.3031	0.386387114	4.347326623	2.190334429
50	1.782953561	12.50422031	0.54446461	-2.63019	0.482983892	5.434158279	2.737920226

A.3 Components of Electrolyser System

Number	Description
1	Water treatment plant including pump and storage tank
2	transformer
3	rectifier
4	Electrolysis stacks
5	Cathode: gas-water separator
6	Cathode: De-Oxidiser
7	Cathode: Heat exchanger (H2 drying)
8	Cathode: Condensate separator
9	Cathode: temperature change adsorption
10	Coolant supply for H2 drying and power electronics
11	Anode: gas-water separator
12	Anode: circulation pump
13	Anode: heat transfer medium
14	Anode: ion exchanger