Review

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Posted Date: 25 May 2023

doi: 10.20944/preprints202305.1786.v1

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Article

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Abstract: In order to harmonize supply and demand of green energy, new future-proof technologies are needed. Here, hydrogen plays a key role. Within the current framework conditions, the production of green hydrogen is not yet economically viable. The use of the oxygen produced and the possible increase in efficiency associated with it mostly remains unconsidered. The aim is to demonstrate that the economic efficiency of a power-to-gas (PtG) project can be increased by using the by-product oxygen. In this research project, a water electrolyser connected to grid is powered to supply hydrogen to a hydrogen refuelling station. By utilising the by-product oxygen from water electrolysis for a wastewater treatment plant (WWTP), it is shown that the net present value (NPV) of the project can be improved by up to 13 % compared to the initial scenario. If a photovoltaic (PV) system is used in addition to grid electricity for higher green hydrogen production, the NPV can be further improved by up to 58 %. The levelized cost of hydrogen (LCOH) is calculated for different scenarios with and without oxygen configuration. A sensitivity analysis is then performed to find important parameters.

Keywords: alkaline water electrolysis; hydrogen; by-product oxygen; wastewater treatment plant; levelized cost of hydrogen; power-to-gas

1. Introduction

With the continuous increase of renewable energy sources (RES) in the power grid, the question of fully efficient use of these energies becomes increasingly important. The biggest challenge here is to balance the supply and demand of energy. With power-to-gas (PtG), the conversion of electrical energy (electricity) into chemical energy (gas) by means of water electrolysis, the renewable energy generated in the electricity sector is made storable in large quantities and can be further used as gas (green hydrogen). In this way, hydrogen can be used as an energy storage system to buffer RES in a supply-oriented and flexible manner and contributes to balancing supply and demand. As an essential element of sector coupling to mobility and the chemical industry, green hydrogen and its downstream products open up new defossilisation paths.

In order to promote the switch from fossil fuels to hydrogen and to achieve the goals of the Paris Climate Agreement, the German government adopted a National Hydrogen Strategy on June 2020 and provided it with an action plan that is to be continuously updated. It describes hydrogen as a "key element of the energy change". [1] So far hydrogen production from fossil fuels has been more economical than production by means of water electrolysis. From the Federal Government's point of

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view, however, only hydrogen produced from renewable energies- green hydrogen is sustainable in the long run. [2,3] In addition, investments in PtG projects require a non-discriminatory regulatory framework and an open market model. In the recent literature on the topic of power-to-X, hardly any attention is paid to the equally important by-product from water electrolysis, oxygen [2,4]. Thus, in most cases it is only mentioned that hydrogen and oxygen are produced from water with the help of electrical energy, although electrolysis produces 8 kilogram of oxygen for every kilogram of hydrogen [5].

The German Hydrogen Strategy aims to achieve a rapid market ramp-up of hydrogen. Domestic production on the basis of renewable energies will have first priority. For a rapid ramp-up and until a cheap supply of green hydrogen can be achieved, the hydrogen regulatory system will be designed in a way that is open to all technologies. An electrolysis capacity of around 10 gigawatts is to be achieved in Germany by 2030, and European cooperation is to be strengthened. [6]. The planned expansion corridor of 137 to 275 GW of installed electrolysis capacity by 2050 in Germany [7] could produce up to 23,000 tonnes of oxygen per hour.

This article proposes to accelerate the expansion of the hydrogen basis promoting the sales of by-produced electrolytically oxygen. This would help to reduce the high electricity consumption in oxygen production by air separation technologies, such as cryogenic air separation or pressure swing absorption [8]. By supporting the market ramp-up in the form of market activation measures, significantly higher electrolysis capacities for storing surplus RES can be achieved, thus also making the purchase of the by-product oxygen interesting. Opportunities must be created to establish hydrogen as a defossilisation option and at the same time to use both products from water electrolysis. There are many markets for PtG. Oxygen is used in the food sector, metal production and processing, recycling, water and wastewater treatment [9–11], waste processing, paper production, the chemical and pharmaceutical industry, in open-cast lakes and aquacultures and in medicine with appropriate purification [5,8,12,13]. Rivarolo et al. [14] for instance, highlights the application of oxygen for use in thermochemical processes such as biomass gasification to produce methane and methanol.

This study aims to demonstrate that the additional use of the by-product from water electrolysis, oxygen, can make the electrolytic production of hydrogen more economical. Various factors play a role in the economically efficient dimensioning the energy system. Some of them include the size and workload of the electrolyser (production capacity), the discount rate/ Weighted Average Cost of Capital (WACC), investment costs, operation costs of the systems, sale price of hydrogen and oxygen. A sensitivity analysis was performed for all the scenarios by varying different parameters in the simulation model to find out the important parameters influencing the economics of the system. It is found that electricity prices play a major role and decide the economic viability of the project.

2. Literature research and overview of simulation software

In general, to produce large quantities of oxygen and other gases like nitrogen and argon, cryogenic air separation units are commonly used. The energy requirement is about 0.464 kWh/Nm^3 of oxygen [15]. Here, the purity of the oxygen produced can be over 99 %, which is why oxygen for medical purposes is usually produced using a cryogenic process due to the high purity requirements. No technique, with the exception of water electrolysis, is expected to challenge cryogenic air separation for the production of large quantities of oxygen in terms of purity. Pure and clean oxygen produced by electrolysis is suitable for medical use. Because of the high price of medical oxygen, effective marketing of this by-product oxygen would reduce the high cost of hydrogen production from electrolysis. [8] When using the electrolytically produced oxygen in wastewater treatment; impurities, which tend to be less than 1 % in electrolysis, basically have no influence [16]. In this case study, the by-product oxygen is used in the wastewater treatment plant as it does not have high purity requirements.

In order to simulate this electrolyser energy system with hydrogen- and oxygen-sided configuration, a suitable simulation software was needed. There are several simulation applications that can be used for the dimensioning of water electrolysers and the simulation of a PtG system. Some of the software programs are: TRNSYS, a software environment used to simulate the behaviour of transient systems. It includes a standard library with various components, also electrolysers [17]. Matlab Simulink is a block diagram environment and can also be used to simulate electrolysers and hydrogen refuelling stations (HRS) [18]. Aspen Custom Modeler is suitable for developing a dynamic model of an electrolyser including a detailed description of the various phenomena involved in the electrochemical process [19]. Aspen Plus contains a variety of standard operation units that can be used, for instance, to evaluate and optimize electrolysis systems for hydrogen production [20]. INSEL is also a block diagram simulation system for programming and visualization of energy systems. The electrolysis-block (electrolysis cell voltage) can be found under the category of the storages [21]. EDGAR belongs to the group of techno-economic simulation and optimization software, also for Power-to-X and sector coupling [22]. EnergyPLAN simulates the operation of national energy systems, including different sectors [23]. In most projects, as described, only the hydrogen product was of interest, which is why previous simulation software for modelling a PtG system with the focus on hydrogen could be used. The path of the by-product oxygen is not included. The oxygen produced simultaneously plays a subordinate role, but can lead to an optimization of benefits in certain areas of application. Especially for the techno-economic design of an electrolyser with hydrogen and oxygen users with diverse requirements, there was no precast solution. This was needed for the project "LocalHy", one of the Hydrogen Power Storage & Solutions East Germany (HYPOS) projects within the BMBF Twenty20 programme [10,11,24–29]. Hence, an innovative software application called GHOST (Green Hydrogen Oxygen Simulation Tool) was developed at Fraunhofer CSP. The user-friendly software application is utilized for this research for all the simulations.

The hydrogen production costs are one of the most important indicators for evaluating such decentralized systems and making them comparable among each other. They represent a constant price over the entire lifetime that would have to be paid by a user for the hydrogen provided in order for the net present value (NPV) of the investment to be exactly zero. Above this price for hydrogen, the investment would have to be valued positively. The greater the production capacity of the hydrogen, the lower the levelized cost of hydrogen (LCOH) [30]. In the study of Minutillo et al. [30] the configuration with the medium system with a capacity of 200 kg/day, 50 % electricity grid reached the lowest value of 9.29 €/kg hydrogen. If the calculations of the hydrogen production costs in the current literature are compared, it can be seen that the liquidation proceeds (residual value of the individual components through sale after the project duration) are not taken into account.

The larger the electrolyser and thus the hydrogen production capacity, the lower the LCOH. In addition, it is found that when no grid electricity is used, the LCOH is also reduced. It is also shown that the LCOH decreases when the project duration is increased [31]. In the same way, the NPV increases when the project duration is increased. Squadrito et al. [32] outlines in his paper the positive influence of the by-product oxygen from electrolysis on the NPV. His results confirm that the oxygen market price, far more than the hydrogen sales price, is the decisive factor for the profitability of the plants studied. Following the calculations in [33] a positive influence of the by-product is predicted, which can help to make the competitive position of green hydrogen comparable with grey hydrogen. In the currently ongoing "Wind Hydrogen" project of Salzgitter AG [34] and in the EU project "GrInHy2.0" (GreenIndustrialHydrogen) [35], the use of hydrogen and oxygen from electrolysis for steel production is being investigated. In addition, the oxygen in the gasification reactor is to be used to produce synthesis gas in the "GreenHydroChem" real laboratory. This can improve the business model for the electrolyser. [36] Moreover, the "Westküste 100" real laboratory will test whether the oxygen also produced during electrolysis can be injected into the combustion process of a regional cement plant with the help of a so-called oxyfuel process, which could significantly reduce the factory's nitrogen oxide (NOx) emissions at the same time [37].

Completed projects that have dealt with the further use of electrolytically produced oxygen at WWTP are the HYPOS project "LocalHy" [10,11,24–29], the project of ARGE Hydrogen Initiative Western Pomerania in Barth [38] and the project "WaStraK NRW" [39]. The potential of WWTP as location for water electrolysers could be confirmed in all projects and offers nationwide

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transferability. Schäfer et al. [40] also describes in his study the positive influence of electrolytically produced oxygen in WWTPs and the role of these in the context of sector coupling.

In **Error! Reference source not found.** the LCOH of different selected publications are listed that show a similar scenario with a water electrolyser as the core. This is either powered by grid electricity and/or solar energy. In some cases, compressors and storage and additional components such as a battery, a pre-cooling system and dispensers with remote monitoring are also included. In order to compare the costs better, all LCOH in the literature were converted into Euros per kg (€/kg). In few publications, very low LCOH values were achieved but without considering all the energy system components. On the other hand, high LCOH values were evaluated for the energy systems with additional components. As hydrogen has to be utlized in a refuelling station in this research, all energy systems have to be considered for techno-economic analysis. The aim is to minimize the LCOH or the hydrogen production costs and hence, oxygen sale is considered as a main pathway to achieve the goal.

Table 1. Comparison of the levelized cost of hydrogen (LCOH) with selected studies.

Literature	Grid	PV	Electro-lyser	Com-pressor & Storage	Additional components	Amount of H_2 produced	Electrolyser size	LCOH [€/kg H_2]
Artuso et al., 2010 [41]		✓	✓			840.15 kg/year	26 kW	17.71
Parra and Patel, 2016 [42]	✓		✓	✓			1 GW	2.55
Ferrero et al., 2016 [43]	✓		✓	✓			10 MW	3.8
Yates et al., 2020 [44]		✓	✓				1 MW	2.39
Grimm et al., 2020 [45]		✓	✓			10.000 kg/day		5.14
Gutiérrez-Martín et al., 2020 [46]		✓	✓	✓	Battery storage	522.8 kg/year	7.97 kW	5.89
Gutiérrez-Martín et al., 2020 [46]		✓	✓	✓		522.8 kg/year	10.9 kW	6.42
Nicita et al., 2020 [5]		✓	✓	✓		12.7 kg/day	180 kW	38.59

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Minutillo et al., 2020 [30]	✓	✓	✓	✓	Refrigeration and H_2 dispensing unit	200 kg/day	472 kW	9.29

3. Methodology

3.1. Model description

The techno-economic system analysis tool GHOST was programmed with Visual Basic for Applications (VBA) in Microsoft EXCEL and can be flexibly extended by additional consumers or functions. Thus, it can be specially adapted to different applications and composition of the components. The data were validated in advance, before being added to the database for the simulation, with real data from the LocalHy project [10,11]. In addition, the numerical model was validated with the freely available energy system simulation tool EnergyPLAN from the Danish University of Aalborg. Here, the operating behaviour of the electrolyser was examined in more detail as a function of the refuelling behaviour [23,26].

Using GHOST, it is possible to model power-to-gas concepts coupled with green or grey electricity on an hourly basis and to determine the optimal system configuration for each individual demand case, both technically and economically [24]. Specifically, for the refuelling of fuel cell vehicles as hydrogen consumers, the CO_2 footprint can additionally be calculated depending on the selected energy. Target values in general are the NPV (NPV > 0, as large as possible), the CO_2 footprint (< 95 g CO_2/km) as a climate value and the number of times the demand is not met as a reliability value. A distinction is made between Priority 1 (simulation stops if demand cannot be satisfied) and Priority 2 (the number of cases and the missing kilograms of hydrogen and oxygen are recorded; the simulation does not interrupt). There are three options for electrolyser operation (continuous operation, only during solar hours and standard operation). [25]

3.2. Detail of system components

In this study, hydrogen and oxygen are produced on-site at a WWTP in Thuriniga, Germany by electrolysis using grid electricity (Scenario 1) or PV electricity generated in-house and supplemented by grid electricity (Scenario 2). In this way, climate-neutral hydrogen for fuel cell electric vehicles (FCEV) can be produced directly at the HRS (here: publicly accessible, for public use). Oxygen can also be used directly in the biological purification stage of the WWTP after intermediate storage, see here **Error! Reference source not found.**. On-site electrolysers offer the great advantage that the refuelling station as well as the aeration basin is independent of hydrogen or oxygen supplies, transport costs are eliminated and the investment costs remain low. Before the hydrogen can be delivered to a vehicle, it must be compressed to the required pressure. The aerator for pure oxygen only works at an operating pressure of approx. 2.5 bar [28]. Therefore, the gas can be depressurized from 90 bar before it is introduced into the aeration tank of the WWTP. The hydrogen and oxygen storage tanks are bundle battery plants in a modular system. This makes it possible to expand existing plants without any problems. The hydrogen refuelling station consists of a high-pressure compressor, a dispenser's pre-cooling unit, a remote monitoring system, a regulation and control system and H_2-dispensers. [47]

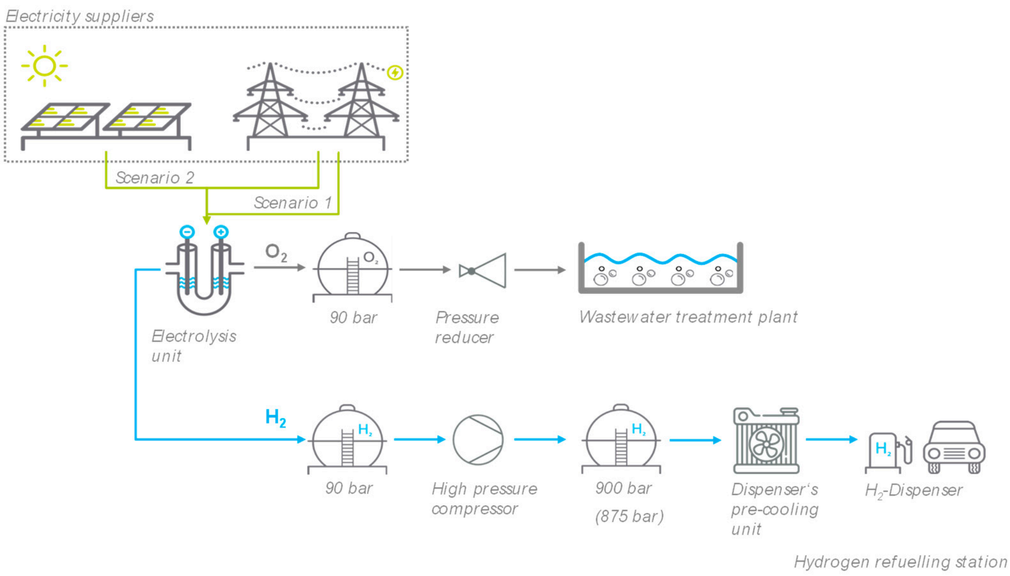

Figure 1. Model of the power-to-gas (PtG) plant with on-site HRS and oxygen utilization in the aeration tank of a wastewater treatment plant (WWTP) at Thuringia, Germany.

The system components to design this model are illustrated below:

a. Electrolyser

The simulation was based on an alkaline high-pressure electrolyser (AEL), which provides the product gases hydrogen and oxygen at a pressure of 90 bar [10,11]. In alkaline electrolysis, the water is usually added at the cathode side (HER – Hydrogen Evolution Reaction), where the hydrogen and the OH^- ions, the charge carriers, are formed. The latter cross the microporous or anion-conducting membrane and are converted to oxygen and water on the anode side (OER – Oxygen Evolution Reaction). The half-cell reaction of alkaline electrolysis looks as follows [48]:

$$\text{Cathode reaction (HER):}\ 2H_2O + 2e^- \rightarrow H_2 + 2OH^-$$

$$\text{Anode reaction (OER):}\ 2OH^- \rightarrow \frac{1}{2}O_2 + H_2O + 2e^-$$

The electrolyser can be scaled as required due to its modular design. The power of the electrolyser for the scenario is 1.125 MW with a hydrogen production of 148,457.43 kg and an oxygen production of 978,768.00 kg. The power-independent losses of hydrogen and oxygen due to, for example, gas measurement or backwashing for gas conditioning and the power-dependent losses of oxygen for water dosing are already deducted here and are taken into account from the outset in the simulation. These can be individually defined by the user of the software. Both gases are initially stored temporarily at 90 bar. In this case study, the hydrogen is then compressed to 875 bar.

b. Photovoltaic system

With the help of a dynamic simulation programme, PV*SOL premium [49], a south-facing ground-mounted PV system was simulated in Sonneberg-Heubisch (Thuringia), the location of the LocalHy project [10,11]. The energy yield of the PV plant generated by the csv-file with hourly resolution is temporarily stored in a separate file by GHOST as an output value and can be linearly scaled in size as required during the system simulation.

According to the ordinance on tendering of Financial Support for ground-mounted systems, there is an upper limit for the size of the offer for a PV ground-mounted system: The offers must each have a size of an installed capacity of at least 100 kWp and at most 10 MWp [50]. For this reason, the maximum size of 10 MWp was fixed as a simulation value. If the average, volume-weighted surcharge value (ct/kWh) is considered over the last few years, the result is an average value of 5,221 ct/kWh. [51]. This was given as the revenue for feeding the remaining PV electricity into the grid in Scenario 2.

c. Oxygen utilization in WWTP

The electricity demand in WWTP could be saved by using pure oxygen from electrolysis. With an average share of 20 %, WWTP are usually the largest consumers of electricity in the municipal sector and consume more electricity than schools, hospitals, administrative buildings or other municipal facilities. The high electricity consumption is due to the aeration of the aeration tank of a WWTP, which usually requires by far the most energy of all the process steps of a municipal WWTP. This is around 50 to 80 % of the total electricity demand of the WWTP. [52] In

the average specific electricity consumption of WWTPs is listed according to the size class. The population equivalent (PE) is defined as the average load of biodegradable substances in the wastewater of a resident. The inhabitant-specific, annual electricity consumption kWh/(PE*a) is used to evaluate and compare the energy parameters. The investigated WWTP is assigned to size class 4. The share of the total electricity demand is 60 % in the study example. The main goal in system optimization of WWTPs is thus to reduce electricity consumption using the oxygen from water electrolysis.

Table 2. Average specific electricity consumption of WWTP by size class according to the Federal Environment Agency. [52].

WWTP size	**Number of inhabitants**	**Specific power consumption [kWh/PE*a]**
Size class 1	< 1,000	75
Size class 2	1,001 - 5,000	55
Size class 3	5,001 - 10,000	44
Size class 4	10,001 - 100,000	35
Size class 5	> 100,000	32

In drainage engineering, a difference is made between the combined system and the separate system. The construction of new sewer networks in the mixed system has largely been completed. All new systems will be separate systems in order not to mix rainwater with wastewater and to divert it separately. In Thuringia there are still predominantly combined sewer systems. [53] Due to fluctuating amounts of precipitation, there is an irregular supply of electrolytically produced oxygen. The wastewater changes over time. Thus, higher precipitation amounts are associated with lower substance concentrations and thus also lower oxygen demand. In the course of time, there are always outliers that require a significantly higher amount of oxygen per hour. This is due to the fact that sudden heavy rainfall events are often accompanied by a so-called flushing surge, which is associated with a high volume of wastewater and high concentrations of substances. This also causes a disproportionately high oxygen demand [54].

Economically, it would be unfavourable to design the entire PtG system according to these outliers, as otherwise the entire system would be oversized and thus could no longer be transferred to economic viability. For this reason, redundancies in the form of oxygen bundles are provided for these cases, which are also considered as additional expenditure for oxygen utilization. Here, the calculation is based on the energy requirement for oxygen from air separation plants, which is offset against the missing quantity of oxygen.

d. Hydrogen refuelling station

 doi:10.20944/preprints202305.1786.v1

SAE J2601 is a refuelling protocol that specifies the requirements of HRS in terms of performance, refuelling process and other operating parameters. The compression process and the refuelling time are also determined here. The latter depends on several parameters, such as delivery pressure (700 or 350 bar), ambient temperature, initial pressure in the vehicle, size of the tank and the degree of refuelling to be achieved. SAE J2601 defines the following parameters as "reference" refuelling values to determine a target for the refuelling time:

- Delivery parameter: 70 MPa @ -40 °C (H70-T40)
- Ambient temperature: 20 °C
- Initial pressure in the vehicle tank: 10 MPa
- Refuelling level to be achieved: 95 %

Under these reference conditions, the maximum refuelling time is set at three minutes. [55] In addition, there is a waiting time until the pump is ready for the next customer (see also **Error! Reference source not found.**).

Different constellations are possible for both off-site (central hydrogen production) and on-site refuelling stations (on-site production). Fraunhofer ISE together with e-mobil BW GmbH (2013) have prepared an overview of various possible HRS concepts. Since off-site refuelling stations are not the focus of this publication, they are not discussed further. [56]. For refuelling stations with decentralized hydrogen production, there are two options for storage and delivery: In cascade refuelling, the gaseous energy carrier flows from the storage tank into the vehicle due to the pressure difference. [57]. In cascading, hydrogen is compressed from the low-pressure to the high-pressure storage tank, if necessary. As soon as a refuelling process starts, the vehicle is filled from the high-pressure storage tank until the pressure is equalized. Hydrogen is then filled from a pressure tank at the next higher pressure. As soon as pressure equalization occurs, a pressure tank with a higher pressure is used. Cascading with as many stages as possible can thus reduce energy losses and is the most sensible solution in terms of energy. However, higher investment and operating costs for the pressure tanks are detrimental to economic efficiency. For this reason, the general conditions are often analysed in cascading in order to determine the refuelling station configuration [58].

In order to achieve a certain refuelling level in the cascade configuration, an overpressure is required. For this reason, hydrogen is usually stored at between 800 and 900 bar in the high-pressure tank. [58–60]. In the case that the refuelling process starts with more than 875 bar (900 bar tank), there is usually a pressure reducer that prevents the pressure from exceeding 875 bar. Therefore, 875 bar was specified as the maximum pressure in the simulation.

In addition, refuelling with a so-called booster compressor is possible. Here, hydrogen is compressed from a low-pressure container directly into the vehicle tank. This publication focuses on cascading.

H2 MOBILITY divides HRS into four broad categories. In **Error! Reference source not found.** the most important parameters that characterize the different sizes are listed. The simulated HRS is a refuelling station of size M - Medium with two dispensers.

Table 3. Parameters of hydrogen refuelling station (HRS) sizes (excerpt) according to the H2 Mobility initiative. [56,61].

	Very small	**Small**	**Medium**	**Large**
Numbers of dispensers	1	1	2	4
Allowed waiting time between two refuelling events in min	20	5	5	0

 doi:10.20944/preprints202305.1786.v1

Max. number of refuelling events per dispenser and hour	2.5	6	**6**	10
Number of refuelling events per day (average/max)	10/20	30/38	**60/75**	125/180
Max. dispensed H_2 in kg/h	18	33.6	**67.5**	224
Dispensed H_2 in kg/d (average/max)	56/80	168/212	**336/420**	700/1000

The hydrogen consumption at the HRS was determined for the simulation with 110,000 kg hydrogen, which is sold for 9.50 €/kg at the refuelling station[1]. This corresponds to about 550 FCEV at an annual average mileage of 20,000 km per vehicle [62]. The hydrogen storage (90 bar) is equipped with 60x50 litre cylinder bundles. This corresponds to a total volume of 3,000 litres (total H_2 stored @ 90 bar: 19.26 kg). The total volume of the hydrogen storage at 875 bar is 24,000 litres (total H_2 stored @ 875 bar: 1,048.30 kg). The present compressor is a hydraulically driven piston compressor that compresses the hydrogen from the 90 bar storage into the 875 bar storage. According to a study by Fasihi et al. [33], hydrogen could be produced on all continents in 2050 at a price of 1.58 €/kg hydrogen. This assumes a reduction in the electricity production costs of renewable energies and an increase in the CO_2 emission licence prices. Furthermore, according to this study, cost degressions of PV plants, wind energy plants, hydrogen compressors and water electrolysers are to be expected up to 2050. Government subsidies, lower investment risks and a lower WACC can also improve local competitiveness [33]. Cost reduction potentials arise primarily from the continuous increase in annual production quantities and the transition to series production.

An increase in utilization cannot be guaranteed by the constellation of electrolyser and storage. Outages may occur, which will not to be considered in this scenario. An increase in the size of the storage facility would also not have had the desired effect. It would have had to be significantly enlarged, which would not have been economical. The focus of this paper is on investigating the influence of the additional use of the by-product oxygen from electrolysis. For this reason, the simulation was set for a 100 % security of supply of around 550 FCEVs with an assumed driven distance of 20,000 km/year. The remaining approximately 38,500 kg of hydrogen in the storage at the end of the year was sold to the surrounding industry for 4.50 € in the present scenario, but could also serve as a buffer in the storage for the new year.

3.3. Levelized Cost of Hydrogen

The LCOH (inferred from the Levelized Cost of Electricity (LCOE)) is considered the most important indicator among the economic valuation indices. Therefore, special attention will be paid to the investigation of these. The LCOH is estimated on the basis of the NPV method. Kuckshinrichs et al. [63] lists not only the LCOH for the cost assessment, but also the NPV for the attractiveness analysis and the variable costs for the analysis of market flexibility.

In the valuation of investments, the NPV method is the most common calculation method. It belongs to the asset value methods and in this sense aims to maximize the final assets. Its result is the NPV, which is calculated from the present value of all cash inflows (E_t) and cash outflows (A_t) of the investment object at time t. CF_t thus represents the net cash flow in the individual periods during

[1] The hydrogen price at the H2 MOBILITY filling stations has risen to 13.85 €/kg H_2 for 700 bar refuelling in June 2022. The simulation still uses the previous price of 9.50 €/kg. [62]

the project term ($t = 1, \dots, T$). The calculation interest rate (equated here with the $WACC$) is given as i and T is the number of periods. If the NPV assumes a positive value ($NPV > 0$), the project is absolutely advantageous and thus preferable to investing money on the capital market. According to the maximization calculation, the project with the highest NPV is therefore relatively advantageous. If, on the other hand, the NPV is negative ($NPV < 0$), investing money in the project proves to be disadvantageous. With a NPV of zero, no advantageous decision can be made using this method, since the return on the investment corresponds to the return on the capital market. In this case, the decision-maker is indifferent to both alternative courses of action. Blohm et al. [64], on the other hand, also see this case as advantageous, since here the desired minimum interest rate is achieved at the calculation interest rate. The NPV formula also shows that the cost of capital increases as the interest rate rises. From this it can be concluded that a higher calculation interest rate causes a lower NPV and thus has a significant influence on it. [64,65] The basic form of the formula of the NPV is as follows [5,64,65]:

$$NPV = \sum_{t=0}^{T} \frac{CF_t}{(1+i)^t} = \sum_{t=0}^{T} \frac{E_t - A_t}{(1+i)^t} \quad (1)$$

In order to further specify this formula, additional parameters are first defined. The payments at the beginning of the project are called initial investment costs (I_0) and do not need to be discounted due to their temporal occurrence in $t = 0$. At the end of the project ($t = T$) the liquidation proceeds (L_T) can be added to the payment surpluses of the last period [66]. The sum of all cash inflows and the liquidation proceeds after deducting the cash outflows results in the net payments. Their cash value in turn leads to the capital value, which is therefore also referred to as the NPV. This can now be represented as [64,65]:

$$NPV = -I_0 + \sum_{t=1}^{T} \frac{CF_t}{(1+i)^t} + \frac{L_T}{(1+i)^T} \quad (2)$$

Inferred from the NPV method, the LCOH with the unit [€/kg H_2] is defined as [30, 64]:

$$\mathrm{LCOH} = \frac{\text{total cost [€]} - \text{electrical revenue [€]} - \text{liquidation proceeds [€]}}{\text{total } \mathrm{H_2} \text{ production [kg]}} \quad (3)$$

$$\mathrm{LCOH} = \frac{\mathrm{I_0} + \sum_{t=1}^{T} \frac{\mathrm{A_t} - \mathrm{REV_{el}}}{(1+\mathrm{i})^t} - \frac{\mathrm{L_T}}{(1+\mathrm{i})^T}}{\sum_{t=1}^{T} \frac{\mathrm{M_{H2}}(1+\mathrm{d_{H2}})^t}{(1+\mathrm{i})^t}} \quad (4)$$

The total expenditure in each period, A_t includes the annual maintenance and operating costs and the annualised replacement cost; M_{H2} is the yearly mass of hydrogen produced, REV_{el} refers to the annual income from the sale (feed-in) of surplus electricity from the PV system to the grid. d_{H2} is the rate of change during the period of time, not only the system degradation rate. d_{H2} can also be positive or negative. For the present calculations d_{H2} was assumed to be zero. If liquidation proceeds accrue towards the end of the project, these must also be considered in the calculation of the $LCOH$. In this project, it is assumed that the individual components reach the end of their service life after a term of 30 years and thus no liquidation proceeds arise in the 30th project year.

$LCOH_{O2}$ with the unit [€/kg H_2] stands for the specific hydrogen production costs, in which the additional revenue from the sale of oxygen was taken into account in each period. The expenses for the additional use of oxygen (e.g. oxygen storage, aeration system) are also included in A_t. The $LCOH_{O2}$ decrease compared to the $LCOH$ only if the expenses for oxygen use are lower than the additional revenue from the sale of oxygen ($E_{t,O2}$). There is a cross-financing of hydrogen production by the revenues of oxygen utilization.

$$LCOH_{O2} = \frac{I_0 + \sum_{t=1}^{T} \frac{A_t - E_{t,O2} - REV_{el}}{(1+i)^t} - \frac{L_T}{(1+i)^T}}{\sum_{t=1}^{T} \frac{M_{H2}(1+d_{H2})^t}{(1+i)^t}} \quad (5)$$

In this example, the revenue from oxygen sales corresponds to the savings in electricity for the blower originally used to aerate the aeration basins. A major advantage of this project is that the electrolytically produced oxygen is already under pressure and therefore no longer needs to be compressed for storage. In addition, there is no need for high-purity oxygen for aeration of the aeration basin, as is the case for medical applications, and thus no purification is required, which does not result in unnecessary costs.

4. Results and discussion

All setting parameters can be found in the tables in the appendix (see **Appendix A**). First, Scenario 1 is discussed, which considers a PtG system that operates only with grid power. Here, a distinction is made between a pure hydrogen application and an additional use of the by-product oxygen. This is followed by an examination of Scenario 2 with its own PV system, which must be procured at the beginning of the project, in addition to supplying the electrolyser with grid electricity. At the end, building on Scenario 2, it is analysed how the sale of oxygen affects the NPV and what influence the WACC has on the result. The whole project time is based on the lifetime of the PV system. The LCOH values with and without oxygen-sided configuration are mentioned in **Error! Reference source not found.**. The best scenario is achieved for the energy system scenario with PV power plant and usage of the by-product oxygen. This scenario has performed well with an LCOH value of 6.28 €/kg H_2. When compared to the selected literature values researched, which are mentioned in Error! Reference source not found., the water electrolyser energy system performed the best due to the additional sale of the by-product oxygen for the wastewater treatment plant.

In order to completely understand the effect of important parameters on the financial aspects of the energy system, a sensitivity analysis was performed by varying four parameters: electricity price, PV power plant specific cost, electrolyser CAPEX and oxygen selling price. The results of the various sensitivity simulations are presented below.

Table 4. Simulation results of the energy system for a scenario without photovoltaic (PV) and a scenario with PV power plant .

Simulation Scenarios	Grid	PV	Electro-lyser	Com-pressor & Storage	Additional components	Amount of H_2 produced	Electrolyser size	LCOH [€/kg H_2]	LCOH O_2 [€/kg H_2]
Scenario 1	✓		✓	✓	Refrigeration and H_2 dispensing unit	407 kg/day	1. 125 MW	7.91	7.44
Scenario 2	✓	✓	✓	✓	Refrigeration and H_2 dispensing unit	407 kg/day	1. 125 MW	6.75	6.28

4.1. Simulation with grid power only (Scenario 1)

In two different scenarios, important factors influencing economic efficiency will be examined in more detail. In Scenario 1, the electrolyser is only operated with grid electricity. A fixed tariff is set here.

4.1.1. Electricity price variation

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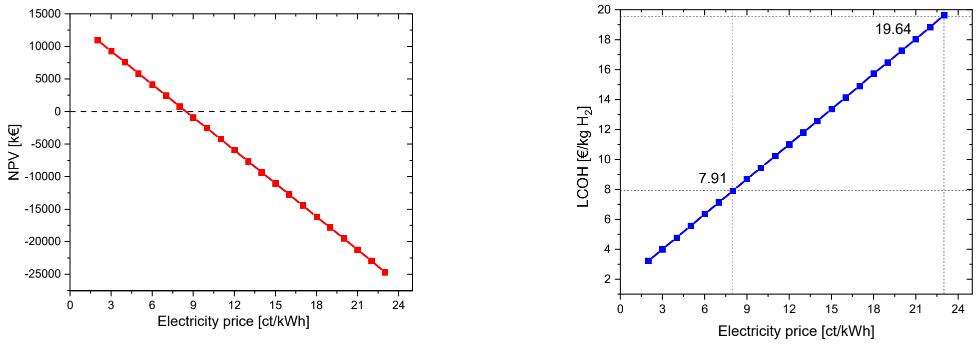
It was found that electricity costs play a major role on the economic efficiency of the overall system. Therefore, this subsection will show how a change in the electricity price helps to bring the PtG system into economic viability, on the one hand for a pure hydrogen use and on the other hand for the use of both products from water electrolysis. The results also show the marginal electricity price at which the project becomes profitable. The electricity price on the x-axis plotted in the following figures always refers to the price for the electricity mix from the grid.

4.1.1.1. Without oxygen use

The initial capital value for the given parameters (electrolysis CAPEX: 700 €/kW and electricity price: 23 ct/kWh) in this example is -25,070.67 k€ for pure hydrogen utilization. The LCOH is 19.64 €/kg H_2. To illustrate the influence of the electricity costs, these were varied from 2 ct/kWh to 23 ct/kWh. At an electricity price of 8 ct/kWh, the NPV achieved a positive result. From here on, the investment in the project is worthwhile. The LCOH reaches a value of 7.91 €/kg H_2. The payback period is 10 years. In **Figure 2**, the NPV and the LCOH are plotted against the electricity price.



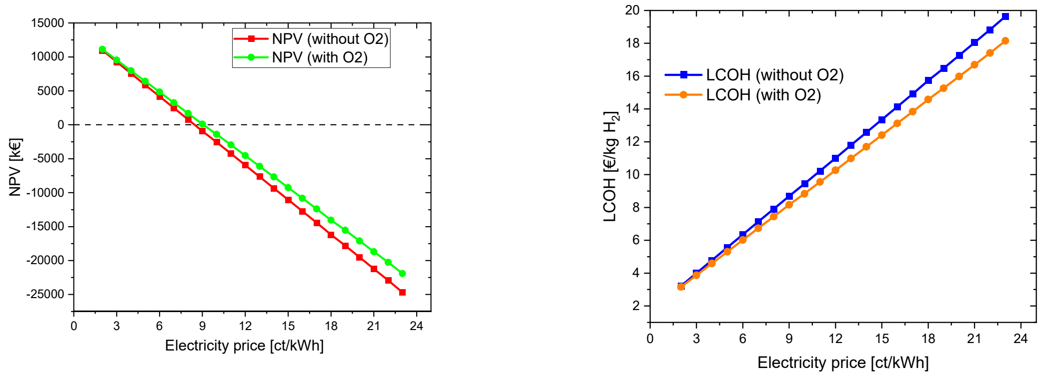
(**a**) (**b**)

Figure 2. Variation in electricity price for a project lifetime of 30 years (**a**) Change in net present value (NPV); (**b**) Change in LCOH values.

4.1.1.2. With oxygen use

If the same settings are used, but oxygen is additionally used for the biological purification stage, there is a slight improvement in the NPV, but it still remains negative: -21,902.37 k€. But for an electricity price of 9 ct/kWh the NPV becomes positive. The LCOH here is 8.16 €/kg and the payback period are 15 years. In order to establish comparability with the simulation in section 4.1.1.1., the electricity price was also set at 8 ct/kWh. Now the LCOH is 7.44 €/kg H_2 and the investment is amortized after only 8 years. **Figure 3** shows the increase in NPV and the reduction in LCOH through the additional use of the by-product oxygen from water electrolysis.

The difference in the LCOH values lies between 0.06 € at an electricity price of 2 ct/kWh and 1.50 € at an electricity price of 23 ct/kWh. The more expensive the electricity is for operating the water electrolysis, the more it is worthwhile to use the oxygen in addition. If it is assumed that the electricity price for accounting for the savings in the aeration tank does not change and is assumed to be constant at 23 ct/kWh, the difference between the LCOH values with and without O_2-benefit is constant at its maximum value of 1.50 €.



(**a**) (**b**)

Figure 3. Variation in electricity price for the energy system with oxygen use for a project lifetime of 30 years, (**a**) Change in NPV; (**b**) Change in LCOH values.

In addition to the NPV and the LCOH, the payback period is another interesting parameter to consider. In **Figure 4**, the payback time of the two cases, with and without oxygen consideration, is listed depending on the electricity price. At an electricity price of 23 ct/kWh, the project duration of 30 years is not sufficient to amortize the project investment. The value here is well over 32 years. In the case with oxygen, the payback period is 15 years at an electricity price of 9 ct/kWh, see above. In order to amortize the investment even in the case without oxygen use, an electricity price of 8 ct/kWh is required. The payback period is 10 years. The strong dependence on the electricity price becomes clear here. The lower the electricity price, the less the two cases differ. This is also confirmed by the NPV and LCOH curves of the two cases, with and without oxygen utilization.

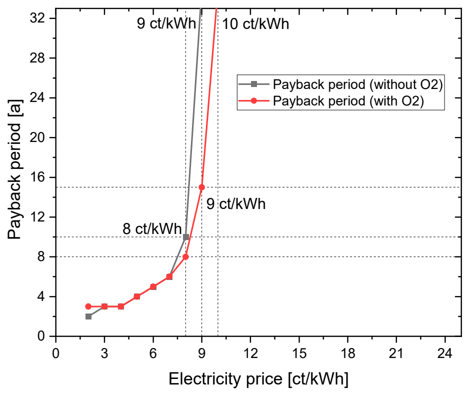


Figure 4. Influence of additional oxygen use on the payback period.

4.1.2. Variation of the CAPEX of electrolyser

In order to additionally investigate the influence of the electrolyser CAPEX (EL) on the NPV, the simulation with oxygen use was selected as the initial scenario. If the NPV is plotted against the electricity costs (see **Figure 5**), there is hardly any difference between the simulations with initial costs of the electrolyser of 200 €/kW to 1,000 €/kW. With CAPEX of 1,000 €/kW, the investment in the project is worthwhile from an electricity price of 8 ct/kWh and lower. For the simulation with electrolyser CAPEX of 200 €/kW to 700 €/kW, the marginal electricity price is 9 ct/kWh. A special case exists for EL = 1,000 €/kW: Here the NPV reaches a positive value in the 19th and 20th year and then becomes negative again. This is due to the fact that several expenses are due in the 21st project year, such as

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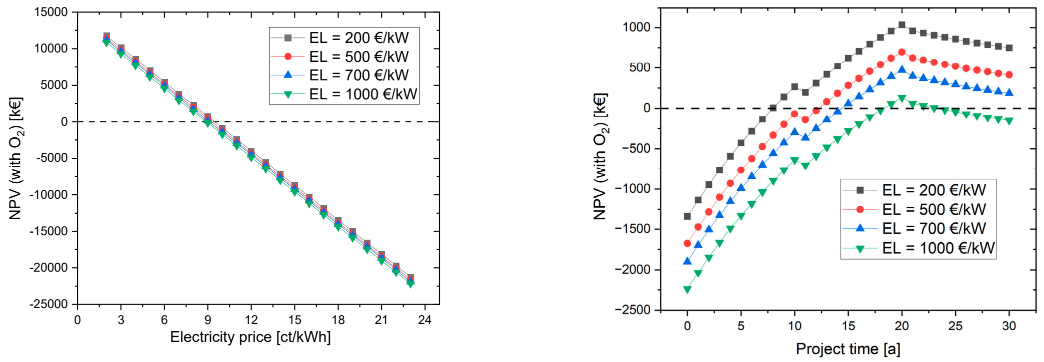
the stack exchange, new contract for the long-term rental of the hydrogen and oxygen storage tanks and also the inspection of the HRS.

In summary, the change in electrolyser CAPEX has a smaller impact on NPV than electricity costs.



(**a**) (**b**)

Figure 5. Effects of varying the electrolysis CAPEX on the NPV (a) depending on the electricity price for a project time of 30 years and (b) depending on the project time with an electricity price of 9 ct/kWh.

4.2. Simulation with grid and PV power (Scenario 2) with oxygen use

The positive influence of oxygen use has already been shown in Scenario 1. Therefore, in Scenario 2, the effects of an own PV system in addition to the purchase of grid electricity (PV+grid) along with the use of the oxygen are considered in particular. If the electrolyser were to be powered only by solar energy, this would not be possible without intermediate storage of the solar energy in a battery. The compressor for the HRS has a system base load, i.e. the compressor must be continuously supplied with electricity even when it is not in operation. A battery could remedy this by providing sufficient power during the night and at times no renewable energy is available. In this scenario, grid electricity was used instead of a battery.

Minutillo et al. [30] found that an optimal configuration is achieved when the annual share of electricity supply from the grid is 50 %. As described in section 3.2. (b), the PV system had to be limited to 10 MWp due to the maximum size for PV systems. For the present constellation of the PtG plant, an annual share of electricity supply by the PV plant of only 35 % is achieved here. However, it can be seen that purchasing electricity from one's own PV system improves the NPV as long as the electricity costs from the grid are higher than 4 ct/kWh (see **Figure 6**). From an electricity price for grid electricity of 12 ct/kWh, the investment in the project is worthwhile. The payback period here is 25 years.

The payback period for the scenario with 100 % grid electricity is 9 ct/kWh over 15 years. If this is compared with the simulation with PV+grid and 9 ct/kWh is also set here, the payback time is 14 years. This is shown in **Figure 7.**

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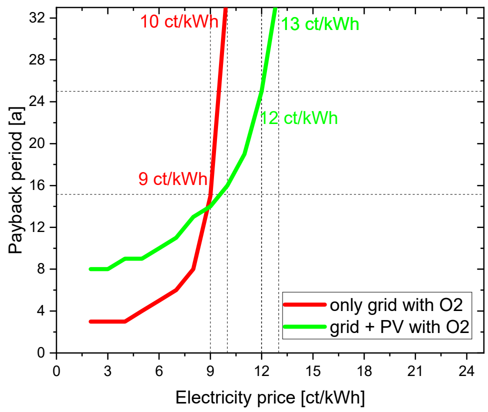

Figure 7. Positive influence of an own PV system on the payback period.

For the project to pay for itself, PV+grid, for example, only requires a reduction in electricity costs to 12 ct/kWh, but if 100 % grid electricity is purchased, an electricity price of 9 ct/kWh is needed for the same result. This shows that PV+grid scenario is more profitable than a complete grid scenario for a 30-year project lifetime even considering additional investment costs of the PV plant.

4.2.1. Variation of CAPEX of the PV system

Currently, the investment costs of the PV module are around 530 €/kWp. A decline in investment costs can make this project financially more profitable. Hence, module prices until 2050 have been considered to investigate and evaluate their effect on the NPV of the project. Fraunhofer ISE conducted a study on behalf of Agora Energiewende and examined the future module prices in different scenarios based on the historical learning curve until 2050. This approach results in module costs decreasing from about 530 €/kWp to 140-210 €/kWp by 2050 in the breakthrough scenario. Other scenarios foresee module prices between 180-260 €/kWp and in the most pessimistic scenario 270-360 €/kWp. [67]

In the best scenario, here 140 €/kWp, an electricity price of at least 17 ct/kWh is needed for the NPV to be more than zero. In the case with 360 €/kWp, the electricity price must be reduced to 14 ct/kWh in order to make the project economically viable (see **Figure 8**). Compared to the studied example with 12 ct/kWh for grid electricity, the future scenario is better.

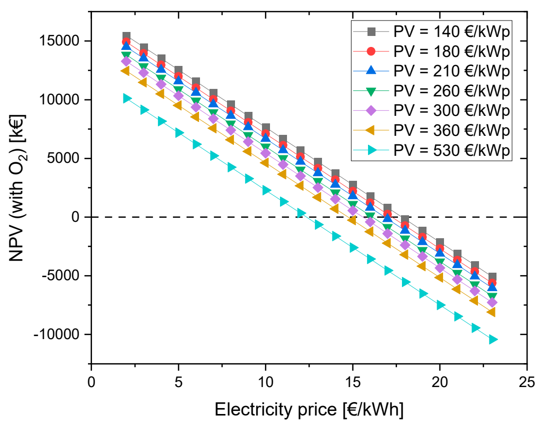

Figure 8. Change in NPV due to variation of PV CAPEX depending on the electricity price for grid electricity.

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4.2.2. Direct sale of oxygen

In the first considerations, oxygen was used in the biological treatment stage to aerate the aeration tank in order to replace the very electricity-intensive blower there. Here, the saved electricity costs were calculated and represented as the financial contribution of oxygen usage. In a further consideration, the oxygen is now to be sold to industry at different prices instead of being reused at the treatment plant. The storage size and costs remain the same to ensure comparability.

If the produced oxygen is sold directly, the project is more profitable for the same electricity price of 23 ct/kWh. All scenarios show profitability in the project as shown in the **Figure 9**, even the scenario O_2 price = 1 €/kg O_2 becomes cost-effective in the 22nd project year. An oxygen selling price of at least 1.50 €/kg O_2 is recommended for this scenario to further increase the NPV. The LCOH decrease significantly, reaching a value of 7.90 €/kg H_2 at 1 €/kg O_2, 4.60 €/kg H_2 at 1.50 €/kg O_2 and 1.31 €/kg H_2 at 2 €/kg O_2. With a different technical composition of the components with different economic parameters, this effect cannot be as pronounced. However, it clearly shows the positive influence of the additional use of oxygen, which is also obtained electrolytically.

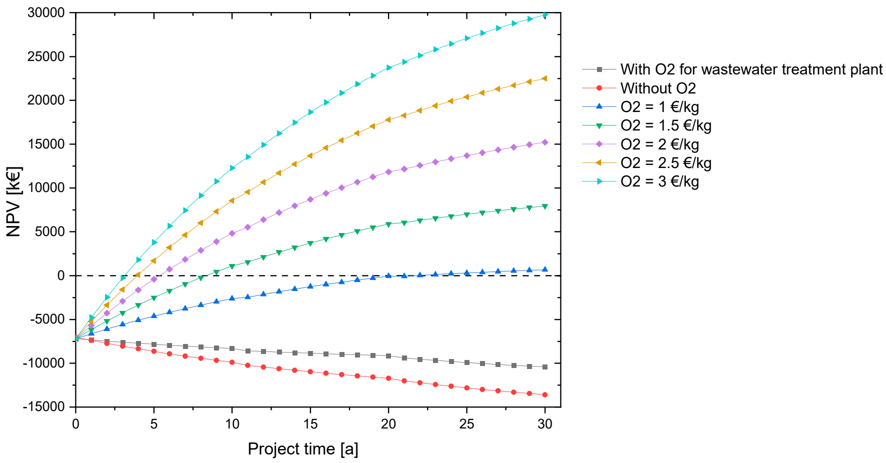

Figure 9. Improvement of the NPV through the additional sale of the electrolytically produced oxygen depending on the project time.

At higher electricity prices for the operation of the water electrolysis, the additional use of the oxygen, which is also produced electrolytically, leads to a greater reduction in the LCOH compared to pure hydrogen use.

4.2.3. Variation of the Weighted Average Cost of Capital (WACC)

Finally, the influence of the WACC (equal to the discount rate) as an important financial indicator and the project time are discussed. The WACC is one of the profitability indicators that have a direct influence on the NPV. It is a valuable tool for business and risk assessment. The lower the WACC, the more positive the influence on the NPV. A longer lifetime also has the effect of improving the NPV (see **Figure 10**). According to the Cost of Capital Study 2020 by KMPG, the WACC for the Energy & Natural Resources sector was 5.3 % in 2020, which was used as the basis for the simulations. [68]

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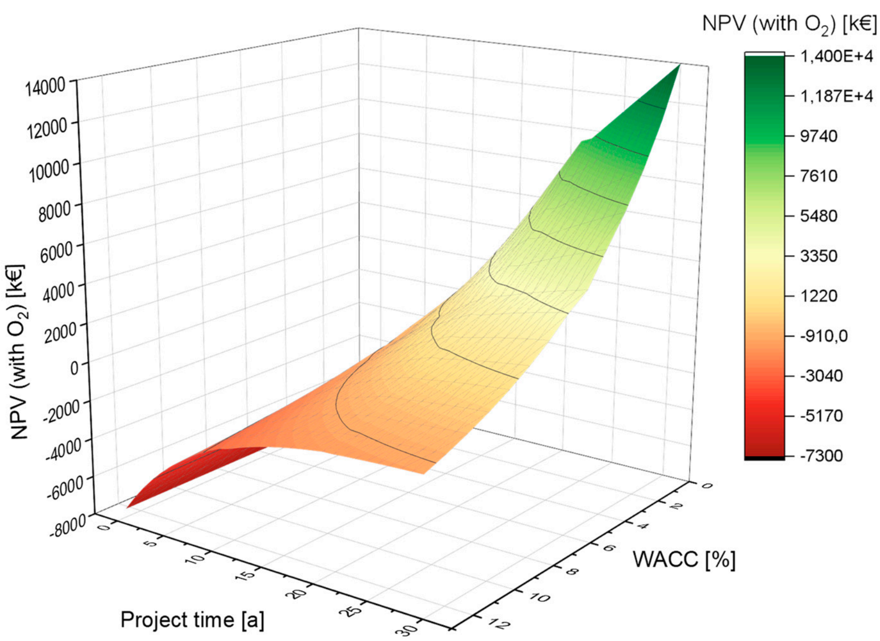

Figure 10. Influence of the Weighted Average Cost of Capital (WACC) on the NPV depending on the project time.

5. Conclusion

A techno-economic optimization was implemented on an energy system containing electrolyser, hydrogen storage, oxygen storage, HRS and WWTP. Sensitivity analysis on different parameters was performed to obtain the best possible case to make the energy system project financially profitable. Two different scenarios were considered in this study: Firstly, the power supply of the on-site water electrolyser with electricity from the grid (electricity mix) and secondly with PV electricity from an own PV system and from the grid.

In both cases, the NPV and LCOH were determined, first only with hydrogen utilization and then with the use of both gases from the electrolysis. The oxygen was used in the biological purification stage of a WWTP. For this purpose, a PV electrolysis system was modelled using the newly developed techno-economic system analysis tool GHOST. In both cases, an improvement in the economic efficiency of the PtG system could be determined through the additional use of the electrolytically produced oxygen.

To confirm the effect of the profitable reuse of the oxygen, another simulation was carried out that examined the sale of the oxygen at different prices. The NPV already reached a positive value in the 22nd project year at a sale price of 1 €/kg O_2. Here it was recommended to set a price of 1.50 €/kg O_2. The operating and maintenance costs are the main influencing factor besides the electricity costs. Therefore, special attention was paid to the variation of electricity costs. A low electricity price can thus have a positive influence on the LCOH value. In addition, it can be assumed that optimization of the components will result in lower acquisition costs and that improvements in the materials will also improve the OPEX.

It is still uncertain how the future electricity system with 100 % renewable energies will look like. As long as the electricity mix still consists of electricity from conventional, controllable power plants, a PtG plant is to be operated for the production of a chemical storage medium (in this case: green hydrogen) in the case of surplus green electricity, this must be available in relevant quantities. The share of RES in the electricity mix must be sufficiently large to achieve profitability. After all, this is the only way the plant can run with sufficiently high full-load hours per year. Furthermore, electrolysis could also act as a provider of balancing power [24]. With positive balancing power, the grid frequency falls below a level that is too low. By switching off electricity consumers, an attempt is made to reduce system load. For example, the PtG plant would have to be switched off or the hydrogen would have to be converted back into electricity using fuel cells or hydrogen-oxygen-combustion engines. In contrast, negative control power results in surplus power that can be compensated for by means of reduced generation output or the ramping up of additional electricity consumers, for example an electrolyser. This scenario could contribute to increasing the full-load hours of an electrolyser without purchasing grey electricity and thus enable economic operation.

Ensuring access to affordable, reliable, environmentally friendly and sustainable energy for all and using resources as efficiently as possible is the foundation of a sustainable economic system. This is to be achieved by Sustainable Development Goal 7 of the 2030 Agenda for Sustainable Development, which was adopted by the United Nations in 2015 [69]. In 2021, a further development of the German National Strategy was even published, as the world is in danger of failing to achieve the goals of the 2030 Agenda [70]. This will help ensure that green energy will be available to everyone affordably in the coming years, including for the production of green hydrogen. Possibly, a green industrial electricity price could be introduced as a transformation turbo for energy-intensive industries to ensure permanently competitive electricity costs. The new coalition in Germany has also promised in its coalition agreement that the economy will get competitive electricity prices for industrial companies, while consistently using its own renewable energy potentials, which it needs on the way to climate neutrality [6]. Chancellor Olaf Scholz's goal would be an industrial electricity price of 4 ct/kWh for Germany. The development of the electricity price is essential for the future of entire industries. [71] The additional use of the by-product oxygen from water electrolysis can effectively contribute to increasing the economic viability of PtG projects.

Supplementary Materials: The following supporting information can be downloaded at: www.mdpi.com/xxx/s1, Figure S1: title; Table S1: title; Video S1: title.

Author Contributions: F. Hönig: Conceptualization, data curation, formal analysis, software, investigation, methodology, validation, visualization, resources, writing - original draft preparation, project administration. **G. D. Rupakula:** Resources, formal analysis, methodology, visualization, writing - review & editing. **D. Duque-Gonzalez:** Resources, data curation, methodology, writing - review & editing. **M. Ebert:** Supervision (general work), funding acquisition, writing - review & editing. **Ulrich Blum:** Supervision (economic work), writing - review & editing.

Funding: This research was funded by the German Federal Ministry of Education and Research, grant number 03ZZ0705D.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

In this appendix, the **Table A.1, A.2 and A.3** show the technical parameters for the simulation, the cost of each component and also the variation of these parameters during the sensitivity analysis.

Table A1. Technical parameters.

Parameter	Value	Unit	References
Project time (Plant lifetime)	30	years	[73]
PV plant peak power	10	MWp	[50]
Total power generation by PV plant	10,427,714.80	kWh/a	[49]
PV degradation rate	0.25	%	[73]
AEL Electrolyser power (without rectifier)	1,125	kW	
Efficiency rectifier	89	%	[11]
Stack lifetime	10	a	[72]
Annual operation	8,759	h/a	

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Deionised water	10	kg/kg H_2	[72]
Hydrogen output[a]	406.8	kg/day	
Oxygen output[a]	2,682	kg/day	
H_2 storage (90 bar)	19.62	kg	
H_2 storage (875 bar)	1,048.3	kg	
O_2 storage (90 bar)	1,417.95	kg	
Long term storage rental	10	years	[11]
System base load compressor	1.25	kW	[47]
Energy consumption per compression operation	60	kWh	[47]
H_2 fixed refuelling volume	110,000	kg H_2/a	
O_2 demand	1,123,142	kg O_2/a	[11]

[a] after deduction of losses

Table A2. Economic parameters.

Parameter	Value	Unit	References
Discount rate (equal to WACC)	5.3	%	[68]
PV plant specific cost (CAPEX)	530	€/kWp	[73]
PV plans OPEX fix	2.5	% of CAPEX p.a.	[73]
Feed-in remuneration for surplus PV electricity	0.05221	€/kWh	[51]
Grid connection cost	1,000	€	[11]
Electricity cost	0.23	€/kWh	[74]
AEL Electrolyser CAPEX[b]	700	€/kW	[7]
AEL Electrolyser OPEX fix	19	€/kW*a	[7]
AEL Electrolyser OPEX var (stack exchange)	45	% of CAPEX every 10 years	[7]
Deionised water	0.01	€/litre	[63]
H_2 storage (90 bar)	22,500	€/10 years	[11]
H_2 storage (875 bar)	180,000	€/10 years	[11] assumption
O_2 storage (90 bar)	90,000	€/10 years	[11]
HRS CAPEX[c]	738,850	€	[47] assumption
HRS OPEX fix	2	% of CAPEX p.a.	[47] assumption
HRS OPEX var (inspection)	2.3	% of CAPEX every 5 years	[47] assumption
Hydrogen selling price at the HRS	9.5	€/kg H_2	[62]
Hydrogen selling price for industry	4.5	€/kg H_2	[75,76]
Aeration system for pure oxygen for aeration basins (CAPEX)	81,024	€	[11]
Aeration system OPEX	2	% of CAPEX p.a.	[11]

[b] all peripheral components (rectifier, electrics, gas equipment, safety system and control system) included

[c] compressor, dispenser's pre-cooling unit, remote monitoring and control system and two H_2-dispensers included

Table A3. Variation of the parameters for sensitivity analysis.

Parameter	Between	and	Unit	References
PV plant specific cost	140	530	€/kWp	[67]
Electrolyser CAPEX	200	1,000	€/kW	[33]
Oxygen selling price	1	3	€/kg O_2	[5]
Electricity cost	0.02	0.23	€/kWh	[71,74]

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