# POWER-TO-X MODELLING WITH IDENTIFICATION OF ECONOMIC KEY FACTORS USING A BUS FLEET SENSITIVITY ANALYSIS

Lukas Saars, Hochschule Niederrhein, +49 2151 822 6676, lukas.saars@hs-niederrhein.de Marius Madsen, Hochschule Niederrhein, +49 2151 822 6697, marius.madsen@hs-niederrhein.de Marc Gennat, Hochschule Niederrhein, +49 2151 822 5112, marc.gennat@hs-niederrhein.de Jörg Meyer, Hochschule Niederrhein, +49 2151 822 6691, joerg.meyer@hs-niederrhein.de

# Introduction

Climate change and the associated need to reduce carbon dioxide emissions (CO<sub>2</sub>-emissions) are increasingly coming into focus of society and politics [1]. International and regional climate targets must be in line with the Paris Agreement in order to limit the global temperature increase to well below 2°C above pre-industrial levels [2]. The Paris Agreement also aims to strengthen countries ability to deal with the impacts of climate change and support them in their efforts [3]. Transport sector is responsible for almost 30 percent of the EU's total CO<sub>2</sub> emissions. As part of the European climate targets, the EU has set itself the goal of reducing transport emissions by 60 percent by 2050 compared to 1990 levels [4]. Thus, one of the key goals of global efforts to reduce greenhouse gas emissions is the decarbonisation of mobility sector. Society has a growing demand of mobility, not only in Europe but also global, transport-related CO<sub>2</sub> emissions are increasing compared to the 1990 reference period, in contrast to other sectors. Fig. 1 shows the breakdown of CO<sub>2</sub> emissions by mode of transport in the EU and illustrates that, in addition to cars, light and heavy duty vehicles account for a large share of total  $CO_2$  emissions [5]. Fig. 2 presents the average greenhouse gas emissions (CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>0 in CO<sub>2</sub> equivalents) by mode of transport in relation to passenger kilometers. In particular, since public buses are rarely used to capacity, they have high specific greenhouse gas emissions [6]. This, and the fact that the use of hydrogen in vehicles can have potential range advantages and shorter refuelling times, are increasingly bringing hydrogen production into the focus of energy suppliers and providers of local public transport. According to a study by the management consultancy Horvath & Partners, 60% of energy suppliers see some potential in the technology [7].



Public transport providers and operators are increasingly influenced by political decisions. The revised European Clean Vehicles Directive promotes clean mobility solutions in public procurement tenders. The new Directive defines

"clean vehicles" and sets national targets for their public procurement. Adopted by the European Parliament & Council in June 2019, the Directive needs to be transposed into national law by 2 August 2021. [8] Therefore, a case study is presented and described in detail at the beginning of this paper. At this point, the model structure, the bus fleet and political and legal framework conditions that have been established in the case study are presented first. The methodical procedure for modelling the electricity market and the system of electrolyzer, hydrogen storage, hydrogen filling station and compressor is then presented. The results of modelling and economic analysis are then described. Finally, in the last chapter, conclusions are drawn and recommendations for action are derived for society and politics.

#### **Illustration of the Case Study**

The use of electrolyzers can play a central role not only for the decarbonisation of regional infrastructures, but also for the offer of flexibilities in the electricity market [1]. Electrolysis of water is the process of using electrical energy from renewable energy sources to decompose water into oxygen and "green hydrogen" [9]. Hydrogen in mobility usually competes with very expensive energy sources such as diesel and petrol. So the use of hydrogen from electrolysis in mobility is a promising path of use. Particularly, due to the shorter charging time and the potentially longer range than a battery electric vehicle (BEV), the focus of local public transport providers is on the use of hydrogen in the heavy-duty sector [10]. Additionally, electrolyzers can use hydrogen storage to offer adjustable options in the electricity market of the future, so that they contribute to the stability of electricity grids. The hydrogen storage system offers the option of taking advantage of favourable electricity prices on the spot market by operating the electrolyzer flexibly [11].

Therefore, the economic viability of using hydrogen as energy in mobility is analysed using the example of a bus fleet. This chapter presents the model structure, consisting of hydrogen infrastructure, bus fleet and the central assumptions on political and legal framework conditions.

#### Model Structure

In the case study, an electrolyzer, a hydrogen fuelling station and a hydrogen storage facility are to be set up to initially supply 10 fuel cell buses with hydrogen. The electrolyzer will be powered with electricity from renewable energies to ensure that green hydrogen is used. It is therefore assumed that the converted hydrogen will not be affected with  $CO_2$  emissions. The components and the assumptions made in this context within the framework of the exemplary model are presented below.

The model uses a polymer electrolyte membrane (PEM)-electrolyzer with an electrical power of 1 MW. This technology was chosen because it is characterised in particular by its ability to operate dynamically and flexibly [12]. Efficiency of PEM-electrolyzers varies between 60 and 75% [13,14,15]. So an efficiency of 71% was assumed without losses due to compression. The information from the literature on the investment for a PEM-electrolyzer also varies greatly, so that a specific investment for the electrolyzer and peripherals of between 900 and 1,800 €/kW should be assumed [11,16]. In the model which described in this paper, 1,520 €/kW is assumed for the specific investment costs. In addition, projects to develop the hydrogen infrastructure are financially supported by national funding programmes in many countries. In model, a funding rate of 40% on the investment for the electrolyzer are assumed to be 3% of the investment sum. In this model stacks have a service life of approx. 80,000 hours and the costs for replacing the stacks in the case study amount to 15.5% of the investment [11,17]. In addition, it is assumed that a water demand of 0.1566 m<sup>3</sup>/MWh<sub>el</sub> occurs for water electrolysis [18]. The water costs amount to 1.50 €/m<sup>3</sup>. The following table summarises the assumptions made in the model.

Electrical power	1	MW
Efficiency [13,14,15]	71	%
CAPEX [11,16]	1,520,000	€/MW
OPEX [11,17]	3	% of CAPEX
Funding rate Investment	40	%
Depreciation period [11]	20	a
Lifetime stacks [11,17]	80,000	h
Stack Replacement	15.5	% of CAPEX
Water demand	0.1566	$m^{3}/MWh_{el}$
Specific water costs	1.50	€/m³

#### Table 2: Assumptions made in the Case Study – PEM-Electrolyzer

The next component in the model is the hydrogen filling station with integrated hydrogen storage and compressor. In this part, gaseous hydrogen is compressed and stored long-term in pressure tanks. Tanks with a pressure of up to 700 bar are now established and commercially available. Pressure storage is an important factor for mobile applications in cars (up to 700 bar) and buses (350 bar) to enable the desired ranges compared to conventional vehicles [19]. In the case study only buses are to be refuelled at 350 bar, so it is assumed that the compressor compresses the converted hydrogen in the filling station to 350 bar. Compression is associated with further efficiency losses and has an efficiency of just under 90% [20,21]. A specific investment of 4,000  $\notin$ /kW is assumed for the compressor [11,20]. The compressor in this case study has an electrical power of 200 kW.

Furthermore, the hydrogen storage tank has a low capacity of 780 kg. The determination of the storage size is discussed in more detail in the course of the paper using economic hydrogen storage size optimization with an mixed-integer linear programming (MILP) problem. The investment of hydrogen storage is set at 630  $\epsilon$ /kg, operating costs are neglected [22]. The further investment for the periphery of the hydrogen filling station, such as dispensing stations, is estimated at 1,000,000  $\epsilon$  [23,24,25]. The following table summarises the assumptions in the case study.

Hydrogen Filling Station		
CAPEX [23,25]	1,000,000	€
OPEX [24,25]	275	€/(kg · a) (daily hydrogen demand)
Funding rate Investment	40	%
Depreciation period [24]	25	a
Hydrogen Storage		
Pressure level [19]	350	bar
CAPEX [22]	630	€/kg
Storage capacity	780	kg
Funding rate Investment	40	%
Depreciation period [20]	25	a
Compressor		
CAPEX [11,20]	4,000	€/kW
Electrical power	200	kW
Efficiency [20,21]	90	%
Funding rate Investment	40	%
Depreciation period [20]	25	a

Table 3: Assumptions made in the Case Study – Hydrogen Filling Station, Hydrogen Storage und Compressor

Finally, the bus fleet represents an essential component that must be described in the following in order to have all elements for the further calculations and modelling. In the model which is described in this paper, 10 fuel cell buses (FCBs) are used and analysed. Electrolyzer, hydrogen filling station, hydrogen storage and depot for the bus fleet are spatially located at a common site, so that the operation of the fuel cell buses does not require any detours. Planning of bus cycles therefore does not need to be adjusted. At the same time, it is assumed in the case study that the refuelling time at a hydrogen filling station is equivalent to the refuelling time at a diesel filling station. This is especially so if vehicles have to be refuelled at frequent intervals, longer refuelling times can occur at hydrogen filling stations [24]. This and the fact that fuel cell buses have to be refuelled more frequently due to their shorter range are neglected in the model.

According to literature, the kilometer-specific hydrogen demand of fuel cell buses varies between 0.08 and 0.12 kg hydrogen per kilometer [19,26,27]. In the model a kilometer-specific hydrogen demand of 10 kg per 100 kilometers is assumed. In addition, the fuel cell buses in the model have an average range of 330 kilometers. Here, the information in the literature varies greatly, so that ranges of up to 500 km can be achieved [26,27]. The lifetime of stacks is 6 years and the cost of replacing stacks is assumed to be  $45,000 \in [17]$ . The buses are depreciated over a period of 11 years and it is determined that each of the 10 buses will cover a mileage of 65,000 km per year. Furthermore, the model takes into account that the battery has a capacity of 36 kWh and must be replaced after 8 years. For the specific costs for battery replacement,  $500 \in /kWh$  was set [28,29]. The potential for cost reduction of cell prices was also taken into account. It was assumed in the model that the investment for a FCB is 650,000  $\in$  and that the innovative share (cost difference to the conventional diesel bus) is supported with a funding rate of 60% [26]. The assumptions made are

summarised in the following table. The assumptions were determined together with a German provider for local public transport.

Number of FCBs in operation	10	
CAPEX [26]	650,000	€
OPEX (kilometer-specific) [26]	0.38	€/km
Kilometer-specific hydrogen demand [19,26,27]	0.10	kg/km
Range [26,27]	330	km
Funding rate on innovative share	40	%
Annual mileage	65,000	km/a
Depreciation period	11	a
Battery capacity [28,29]	36	kWh
Lifetime battery [28,29]	8	a
Specific costs battery replacement [28,29]	300	€/kWh
Lifetime Stacks [17]	6	a
Stack-Replacement [17]	45,000	€

Table 4: Assumptions made in the Case Study – Fuel Cell Buses

The investment and operating costs for the conventional diesel buses were taken into account in the economic efficiency calculation. In addition,  $CO_2$  prices were also assumed, so that the  $CO_2$  price over the period under consideration averages 40  $\epsilon/t$ . This results in rising diesel prices, which are also taken into account in the profitability analysis. The following assumptions were made in the case study. The assumptions were all made together with a German provider for public transport that plans to use fuel cell buses.

Table 5: Assumptions made in the Case Study – Diesel buses

CAPEX	240,000	€
OPEX (kilometer-specific)	0.295	€/km
Kilometer-specific diesel demand	0.35	L/km
Range	500	km
Annual mileage	65,000	km/a
Depreciation period	11	a
Specific costs for Diesel as fuel	0.90	€/L

# Political and legal framework

The worldwide efforts to integrate hydrogen as energy into the global markets are evident in the political decisions and resolutions of many nations. Many countries have now published national hydrogen strategies. As a study by Deutschland e.V. in cooperation with the World Energy Council shows, the strategies differ in their degree of concretisation, focus, goals, measures and level of ambition. To this end, the World Energy Council examined current developments in greater depth in the study "International Hydrogen Strategies". In particular, the study analysed the hydrogen strategies and examined, which packages of measures they contain. The study came to the conclusion that policy should focus on the commercialisation of hydrogen infrastructures [30].

Political decisions of international climate targets have a significant influence on developments in the hydrogen sector and the associated expansion of electrolysis capacity. Funding of investments in the hydrogen infrastructure is becoming increasingly important worldwide. Therefore, funding quotas based on concrete funding programmes are also assumed in the model, which is described in the case study. The corresponding funding rates were already described in the previous chapter.

At the same time, regulatory measures also play a central role in integrating water electrolysis into global energy markets. The following diagram was drawn up based on the study by Deutschland e.V. in cooperation with the World

Energy Council described above and shows that most nations focus on R&D support, regulatory measures and financial support in their hydrogen strategies.

Support	EU	DE	NL	FR	ES	IT	UK	NO	RU	JP	KR	CN	AU	МО
measure type					<u>.</u>						<b>*</b> •*	*1	*	*
R&D support	++	++	++	++	++	+	++	+	++	++	++	++	++	++
Regulatory measures	++	+	++	+	++	+	+	+	+	++	++	++	++	+
Financial support	++	++	++	+	++	+	+	+	+	++	++	++	++	+
Acceptance and training	+	+	0	+	+	0	0	+	0	+	+	0	++	0
Governance and other	+	++	+	+	+	+	0	0	+	++	++	0	++	0
*++ Strong focu	*++ Strong focus, + less pronounced, O not mentioned													

Fig. 3: Support Measure Types in Global Hydrogen Tragedies [30]

In addition, the price of electricity also has an enormous influence on the economic viability of an electrolyzer with hydrogen storage and filling station. In Germany, for example, the "National Hydrogen Strategy" will examine whether the electricity used to produce green hydrogen can be largely exempted from taxes, levies and surcharges. Not only Germany, but also many other nations are planning political and regulatory measures to exempt the electricity used to produce green hydrogen from taxes and levies. This confirms the assumptions made in the model. The model assumes an electricity price of 67.20 €/MWh for the electricity used in water electrolysis.

### **Methodical procedure**

# Economic hydrogen storage size optimization with MILP

For the transferability of the results to all constellations of electrolyzer nominal power and storage size, the unit (electrolyzer) full load hours is introduced in the following. For example, if an electrolyzer can produce 1 kg hydrogen per hour, the associated storage with an exemplary storage size of 10 kg  $H_2$  is equivalent to a storage size of 10 full load hours.

To determine the cost-optimal electrolyzer operation mode to compute the optimal electricity price forecast, the problem is formulated as an mixed-integer linear programming problem, whereby the given example in (1) is relaxed to an ILP. Referring to traveling salesman problems [31], a similar approach is used. The objective function is formulated with

$$J = \min_{x} c^{T} x, \qquad c \in \mathbb{R}^{n}, \ x \in \mathbb{Q} \ [0 \le x \le 1]^{n},$$
  
subject to  $A \cdot x \le b \qquad A \in [-1,0,1]^{m \times n}, \ b \in \mathbb{R}^{m}$  (1)

whereby *n* represents the number of hours *h* in the year times the number of constrains und m represents the number of days. Binary decision vector is noted as *x* with length X = H, and *c* contains the hourly exchange electricity prices. Inequality constraints of this integer linear program can be passed to the solver as *A* and *b*. Because the inequality constraints specifies that  $A \cdot x$  is less than or equal to *b*, the contents of *A* and *b* are negated in the following to invert the constraints. For the first day,  $A_1$  is filled with -1 in row one and columns one to 24.

Ten full load hours of the electrolyzer are required per day  $(b_{1_1}=-10)$ . Therefore, 20 full load hours are required in two days  $(b_{1_2}=-20)$ . The constraints  $A_1$  and  $b_1$  ensures that at least 10 full load hours occur on the first day, at least 20 on the first two days and at least 30 on the first three days.

It is assumed, that the quantity of hydrogen, which has to be refueled the next day, is always taken from the tank promptly at midnight. Constraints  $A_2$  and  $b_2$  ensure that the hydrogen storage has a finite capacity. In this example, the storage tank has a capacity of 50 electrolyzer full load hours. Because 10 full-load hours are refueled by buses on each day, the electrolyzer should produce 60 full-load hours on the first day ( $b_{21} = 60$ ) from storage perspective.

		d	= 1			d =	2			d =	3			
h =	1	2		24	25	26		48	49	50		72		
	/ 1	1	1	1	0	0	0	0	0	0	0	0\	( 60 \	
$A_2 =$	1	1	1	1	1	1	1	1	0	0	0	0)	$b_2 = (70)$	(3)
	$\setminus 1$	1	1	1	1	1	1	1	1	1	1	1/	\ <sub>80</sub> /	

 $A_1$  and  $A_2$  are concatenated vertically to A, and vectors  $b_1$  and  $b_2$  to b respectively to hand A and b over to the MILP solver.

This mixed-integer programming leads to the most favorable electrolyzer operation. In Fig. 4 the H<sub>2</sub> level is shown for an exemplary storage with a capacity of 50 full-load hours over 30 days.



Fig. 4: H<sub>2</sub> Storage Level with Economical Optimal Electrolyzer Operation

To determine the economical optimal storage size, this optimization is carried out iteratively for different storage sizes and compared in each case with the specific costs of the respective storage.

#### Dynamic investment calculation

In dynamic investment calculation, all cash flows are differentiated over time, combined with a calculation of interest. The use of dynamic methods is based on a very detailed consideration.

The net present value (NPV) indicates the present value of an entire investment project, consisting of the sum of its particular values. A particular value represents a discounted period balance of an investment calculation model and thus the present value of a single period.

The net present value is therefore the value that all future cash flows have in the present. The NPV was used to assess the profitability. For this purpose, the following formula (4) was used, taking into account the residual values [32]:

$$NPV_{0} = -I_{0} + \sum_{t=1}^{n} \frac{C_{t}}{(1+i)^{t}} + \frac{R_{n}}{(1+i)^{n}} \qquad \begin{array}{c} I_{0}: \text{ Investment} & n: \text{ Investment period} \\ C: \text{ Cashflow} & i: \text{ Calculation interest rate} \\ t: \text{ Time interval} & R: \text{ Residual value} \end{array}$$
(4)

The period under consideration is twenty years and a depreciation period of 25 years is assumed for the electrolyzer and the hydrogen storage. In this business case, the stack replacement costs were taken into account as operation an maintenance costs. The following example shows how a net present value calculation can be performed.

Table 6: Structural set-up of the net present value method in the case study

End of period	0	1	2	3	 Т
Interest Rate it		4 %	3 %	5 %	
$q_t = (1+i_t)$		1.04	1.03	1.05	
Cash Flow 1	-1,000€	-500€	-100 €	-50 €	
Cash Flow 2		1,000€	1,000 €		
Total Cash Flows	-1,000€	500€	900 €	-50 €	
Particular-Value <sub>T</sub> (numeric)	-1,000€	481€	840 €	-44 €	
Particular-Value <sub>T</sub> (formal)	$=\sum Z_0$	$=\sum \frac{Z_1}{q_1}$	$=\sum \frac{Z_2}{(q_1 \times q_2)}$	$=\sum \frac{Z_2}{(q_1 \times q_2 \times q_3)}$	 
NPV	276.49 €				

In addition to the electricity price of 65.83 €/MWh, an calculate interest rate of 6.50% was assumed to calculate the present values of the periods.

The mass-related production costs are also calculated as part of economic efficiency analysis. The calculation is also dynamic, so that the costs are set in relation to the converted quantity of hydrogen over the entire runtime [33]:

$\sum_{t=1}^{n} \frac{L_t}{(1+i)^t}$	LCOE: Levelized cost of energy	n: Investment period
$LCOE = \frac{(1+1)}{\sum_{n} E_t}$	<i>i</i> : Calculation interest rate	C: Total costs
$\sum_{t=1}^{\infty} \overline{(1+i)^t}$	E: energy generated (in this case hydrogen)	<i>t</i> : Time interval

#### Sensitivity Analysis

The use of sensitivity analyses enables a critical comment on the results of economic efficiency calculations. In particular, the effects of changes in parameter settings are visualised and clarified. Sensitivity analyses enable a statement on influence of changed parameter settings on the result of economic efficiency analysis. This is recommended in practice in order to be able to correctly classify individual parameters. For this purpose, assumed values for the influencing factors are lowered by 25 repectively 50% and increased by 25 repectively 50% and the NPV is determined again after changing the parameters. This makes it possible to identify the influencing factors with a significant impact on the result of the economic efficiency calculation [34]. In addition, statements can be made about the essential adjusting screws in order to derive recommendations for action for society and politics.

#### Results

# Design and dimensioning of the hydrogen storage tan

The mean value of the German electricity prices at European Energy Exchange (EEX) over the exemplary entire year 2019 was about 37.7  $\notin$  per MWh [35]. The following diagram describes the average exchange electricity prices that can be achieved in the best case, depending on H<sub>2</sub> demand and storage size.



If the electrolyzer has to operate less than 24 hours per day, there is some potential by avoiding timespans with high electricity prices. Installing an electrolyzer capable of providing two times the demand would have saved about  $7 \notin$  per MWh in 2019. However, a larger electrolyzer also increases the investment amount to a large extent. The same problem arises when increasing the H<sub>2</sub> storage. Depending on the electrolyzer design, up to  $2 \notin$  per MWh can be saved with a large storage, which is shown in Fig. 5. This requires a huge storage, which results in a high investment. In addition, an ideal electricity price forecast without any deviation for the whole year is needed to achieve this result.

An electrolyzer and a hydrogen storage should always be designed closely to the demand, because the higher investment by higher dimensioning of electrolyzer and storage probably cannot be compensated by the electricity price savings.

For further consideration, taxes and levies must be taken into account. It must also be clear that the achievable electricity price shown in Fig. 5 represents an optimum under ideal conditions.

# Levelized Cost of Energy and Net Present Value

In the model presented, LCOE as well es NPV is calculated. The assumptions made in Chapter "Illustration of the Case Study" result in mass-based hydrogen production costs of  $5.60 \notin$ /kg. The residual values for the electrolyzer and hydrogen storage were also taken into account in the calculation. The components of the LCOE calculation are shown in the following diagram.



Fig. 6: Levelized Cost of Energy Calculated in the Case Study

The economic efficiency calculation take into account the investments as described in the chapter "Illustration of the Case Study". The avoided costs for the acquisition and operation of the fuel cell buses in the period under consideration are implemented. These include in particular the acquisition costs and operating costs (diesel as fuel) of the diesel buses. For the assumptions made, the NPV shown in Fig. 7 result with the key factors and sensitivities. The result shows that despite high subsidy rates (40% for electrolyzer, fuelling stationand, H<sub>2</sub>-storage and for FCEBs on the innovative share) the NPV results clearly in negative values. The electricity price components such as levies, grid fees and taxes have a huge influence on the NPV-result.

The model calculated a net present value of  $-6,714,511 \notin$  over the observation period of 11 years. In the model, the use via fuel cell buses is considered. The products heat and oxygen, which are often classified as by-products, are thus neglected in the economic efficiency calculation. The hydrogen demand that must be served by the electrolyzer results from the specified annual mileage of the buses of 65,000 km. The electrolyzer with a capacity of 1 MW was designed larger in order to be able to react to dynamic developments through the potential expansion of the fleet.

In the model described in this paper, the electrolyzer achieves approx. 3,554 full load hours under the assumption that ten fuel cell buses are used, and thus converts 65,000 kg of hydrogen per year. In addition, compared to conventional diesel buses with the same mileage, approx. 603 tonnes of CO<sub>2</sub> are saved per year. Sensitivity analyses are performed to identify and evaluate those factors that have a significant influence on the result of the net present value method and the hydrogen production costs. For this purpose, four influencing factors are considered and varied upwards and downwards in steps of 25% and 50%. The following table presents the assumptions of the base case.

#### **Table 7: Basis for Calculating Sensitivities**

Key Factors		Value -50%	Value -25%	Base Case	Value +25%	Value +50%
Diesel Price	[€/L]	0.45	0.68	0.90	1.13	1.35
Hydrogen Demand per Kilometer	[kg/km]	0.05	0.08	0.10	0.13	0.15
Exchange Electricity Price	[€/MWh]	20.96	31.43	41.91	52.39	62.87
Price for Carbon Dioxide Emissions	[€/t]	20	30	40	50	60

With an increase of the electricity price by  $67.56 \notin$ /MWh, which roughly corresponds to the levy based on the renewable energy law in Germany, the NPV is reduced by 1.91 mio.  $\notin$  from -6.71 mio.  $\notin$  to -9.18 mio.  $\notin$ . Furthermore, Fig. 7 shows that the diesel price (fuelling of the diesel buses as a comparison scenario), the kilometer-specific hydrogen demand of FCEBs as well as the exchange electricity proce have a significant influence on NPV-results. In addition, the price increase for CO<sub>2</sub>-emissions does not have a major impact.



Fig. 7: Sensitivity Analysis - Significant Factors Influencing the Net Present Value (NPV)

# Conclusion

This paper illustrates that, above all, the price of  $CO_2$ -emissions must rise in order to increase the economic viability of the technology of water electrolysis. At the same time, the electrical power used in electrolysis must be largely exempt from grid fees, taxes and levies in order to be able to increase NPV significantly. Other factors with a positive influence on NPV are price reductions for electrolyzer, storage system and FCEBs.

Furthermore, modelling of the hydrogen storage shows that at current prices for the hydrogen storage system, it is not reasonable under the assumptions made to build a large storage facility in order to use flexibleness on the power exchange. This does not yet take into account a possible participation in the balancing energy market, which could be considered in further investigations.

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